REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*

2. REPORT TYPE
Final Report

3. DATES COVERED *(From – To)*
01-Jul-03 - 01-Oct-05

4. TITLE AND SUBTITLE
High Temperature Magnetic Shape Memory Ni-Mn-Ga Alloys for a New Class of Actuators and Sensors

5a. CONTRACT NUMBER
STCU Registration No: P-137

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
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5d. PROJECT NUMBER

5d. TASK NUMBER

5e. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT NUMBER
N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
EOARD
PSC 821 BOX 14
FPO 09421-0014

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
STCU 00-8011

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
This report results from a contract tasking Institute for Metal Physics as follows: This project will conduct a fundamental study of Ni-Mn-Ga-X alloys exhibiting large and stable values of magnetic-field-induced strain at temperatures above 320 K. The objective is to establish the factors determining the values and stability of magnetic shape memory behavior in order to feed the design of a new class of magnetic shape memory actuators and sensors. Specifics of the project are: (i) the complex theoretical and experimental study of a correlation between electronic, magnetic, and crystalline structure and the phase transformation temperatures with occurrence of magnetic shape memory effect (MSME) using various experimental techniques and theoretical calculations in an attempt to determine the physical grounds for design of MSME alloys; (ii) a study of phase, thermal, and mechanical stability of martensite and the corresponding magnetic-field-induced strain in studied Ni-Mn-Ga and Ni-Mn-Ga-X high temperature magnetic shape memory alloys.

15. SUBJECT TERMS
EOARD, Materials, Metallurgy and Metallography

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18, NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UNCLAS	UNCLAS	UNCLAS	UL	55	JOAN FULLER
					19b. TELEPHONE NUMBER *(Include area code)* +44 (0)20 7514 3154

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

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Project's starting July 2003- project's ending July 2005
Financing parties: USA, European Office of Aerospace Research & Development (EOARD)

Reported period: report's starting: July 2003 - report's ending: September 2003
Date of the report submission: 10 October 2003

Content of quarterly progress report for Quarter 01

1. Summary of progress.

Stage number and title	*1. Theoretical and experimental study of Ni, Mn, Ga contents influence on the phase transformations, electronic and crystal structure, magnetic properties and strain induced by magnetic field*
Actual progress	By means of spin polarized band-structure LAPW calculations, electron structure of Heusler alloy Ni_2MnGa in cubic modification was studied (sub-stage # 1.1) Data about energy band structure of alloy, total and partial electron densities, magnetic moments on atoms, electron densities on Fermi level, contributions of different symmetry type electrons to electron thermal conductivity of substance Ni_2MnGa in cubic modification were obtained. According to the sub-stage # 1.8, X-ray fluorescent emission spectra of the martensite and austenite phases of the alloy Ni50.5Mn28.2Ga21.4 possessing giant magnetic shape memory effect were obtained

using SARF-1 device. Interpretation of experimental data was carried out by comparison with results of electron band structure calculation.

According to the plan of the 1st quarter (stage 1.2-1.7), the influence of changes in the Ni, Mn & Ga concentrations on the phase transformation temperatures, martensite crystal lattice type and magneto-plasticity were investigated. Obtained results are essential for determination of the optimal Ni-Mn-Ga composition possessing magnetic shape memory effect since that is the goal of the project.

8 polycrystalline ingots of non-stoichiometric composition with different Ni, Mn & Ga content (stage #1.2) were melted. The composition of the produced alloys lies in the Ni- (46,3-53,3%), Mn- (19,1-31,5%) , Ga- (16,1 –29,7%) (atomic %) interval.

Since there is loss of Mn content in the alloys composition at high temperatures, we performed studies of the effect of high-temperature specimen treatment (i.e. melting, homogenization, aging for ordering and growing the single crystal from polycrystalline ingot) on the chemical composition of the alloys (phase #1.2). Chemical composition investigations were performed after each stage for two selected alloys. According to performed studies, 1.6-2% of Mn content is lost compared to the furnace charge composition while melting. Due to homogenisation and aging for ordering up to 2% Mn content is lost. Single crystal growth leads to losses up to 2.5% of Mn depending on the speed of cooling. Thus resulting chemical composition significantly changes due to high-temperature treatment of specimen, leading to strong changes in the phase transformation temperatures. Temperatures of phase transformations were investigated for 15 alloys compositions in polycrystalline state after homogenisation and aging for ordering, as well as in single crystals after the same treatment procedures (phase #1.3). Following tendencies are determined:

(i) increase of Ga (28-30%) concentration instead of Ni (48-47%) with Mn =23-24% leads to the increase in the temperatures of phase transformation (M_s= 53^0C, M_f=45);

(ii) simultaneous increase in concentrations of Ni (53.3%) and Ga (27.6%) instead of Mn (19%) leads to growth of temperature of martensite phase transformation (M_s= 84^0C, Mf= 77^0C);

(ii) increase of Ni (53.5%) concentration at expense of Ga (22%) with Mn 25.6% results in significant rise of martensite transformation temperature (M_s= 192^0C, M_f= 185^0C);

(iii) rise in Mn (29-30%)content instead of Ga (18-21%) and Ni (48-49%) causes decrease in the martensite transformation temperatures. (Ms= 24-32^0C, Mf= 20-29^0C).

Alloy Ni49.7Mn28.7Ga21.6 revealing giant magnetic shape memory effect (5.6%) under room temperature has martensite-austenite transformation temperatures of: Ms= 32^0C, Mf= 29^0C, A_s=38^0C, A_f=41^0C.

The effect of change in the chemical composition on Curie point is inessential. In the interval of concentrations of Ni-Mn-Ga alloys mentioned above, Curie temperature lies in the interval of 91-108^0C.

Based on the elaborated single crystal growth technique parameters (temperature diagram, cooling/heating speed etc) (phase #1.4), 3 single crystals were grown (26-32 grams) from selected polycrystalline ingots. We will continue elaboration of the optimal crystallisation technique to improve the single crystal quality.

4 compositions of the produced alloys with higher martensite transformation temperatures were chosen for further studies:

(A) Ni50.5Mn28.2Ga21.4 (A_s=41^0C, A_f=46^0C);
(B) Ni51.4.Mn27.6Ga21 (A_s=75^0C, A_f=82^0C);
(C) Ni53.3Mn19.1Ga27.6 (A_s=88^0C, A_f=93^0C);
(D) Ni52.4Mn25.6.2Ga22 (A_s=151^0C, A_f=161^0C).

Alloys A, B, C were investigated in a single crystalline and alloy D – in a polycrystalline state. According to the magnetisation studies, all alloys have strong magnetic anisotropy (phase #1.6).
Crystal structure of martensite (phase #1.5) strongly depends on Ni, Mn and Ga concentrations. Alloy A was determined to have orthorhombic 5-layered modulated structure of martensite, which remains stable in the temperature interval from start of the martensite transformation until -193^0C. Alloy B has orthorhombic 7-layered modulated structure during cooling from 74^0C down to 15^0C. Alloys C and D have tetragonal non-modulated martensite structure, which remains stable from start of the martensite transformation until room temperature.

Alloys having non-modulated tetragonal martensite do not seem to have any magnetic field induced strains in fields up to 1.2T. Alloy A with 5-layered martensite structure possesses magnetic field induced strains up to 5.4-6% in field below 0.7T in temperature interval from room up to 38^0C (p.#1.7).

The theoretical investigation of the maximal and reversible strain values under simultaneous contrary (perpendicular) application of magnetic field and compressive mechanical stress (p.#1.9) was started using the statistical theory approach being developed by project participants.

2. Summary of personnel commitment.

Investigation of the electronic structure (sub-stage p.#1.1 & #1.8) were performed by I. Urubkov (experimental investigation of the etalon specimens Ni, Mn, Ga and alloy A) and V.M. Uvarov (numerical calculations of the obtained spectra).

Work by sub-stage #1.2 were performed by N. Glavatska (selection of the alloys chemical composition and procedure of thermal treatment), V. Cherepin (local chemical analysis), V. Bliznyuk (melting of the polycrystalline ingots), A. Urubkov (specimen preparation, melting of the polycrystalline ingots), E.Tarusin (thermal treatment), I. Bojnitska (orientational analysis of poly- and single crystalline specimens by X-ray texture analysis method). For chemical analysis of melted alloys V.Didyk was invited, which though is not a project participant.

Stage p. #1.3 was performed by A. Urubkov (determination of phase transformations temperatures by dilatometry method), I.Glavatskyy (determination of phase transformations temperatures by tenso- and magnetometry methods), A.Dobrinsky (determination of phase transformations temperatures by low field magnetic susceptibility method), N.Glavatska (phase analysis by X-ray and neutron diffraction methods), I.Bojnistka (X-ray diffraction phase analysis).

Single crystal growth and technique development (p. #1.3) was done by I. Zasimchuk and L. Matvienko.

Magnetic properties (magnetisation, magnetic anisotropy) of the selected alloys (p. #1.5) were investigated by I. Glavatskyy.

Austenite and martensite crystal structure (p. #1.6) were studied by I. Bojnitska (X-ray diffraction study of the polycrystals), G. Moghylny (X-ray diffraction studies of the single crystals), I. Glavatskyy (neutron diffraction studies of the single crystals), N. Glavatska (neutron diffraction study of the single and polycrystalline specimens).

Magnetic field induced deformations (p. #1.7) were investigated by A. Urubkov and I. Glavatskyy.

Theoretical studies f the magneto-mechanical behaviour of magnetic shape memory alloys (p.#1.9) was performed by V. Lvov, N. Glavatska and O. Rudenko (mathematical modelling).

According to the 1st quarter work plan (p.#1.10) was provided technical maintenance and modernisation of the 3-circle X-ray diffractometer (goniometer was repaired and modified). The work was done by G.Moghilny (calibration, adjustments, tests), M. Knysh (prophylactics and repair of the water cooling system, mechanical works). For construction and manufacture of the new parts for goniometer, we invited A. Marunyuk and O.Rasumov, though they are not project participants. Their work was paid according to the p. #6, Table. 7, Annex. 1. Technical specifications and principal construction for creation of the temperature control and stabilisation system for X-ray studies at high temperatures was created by N. Glavatska, E.Bersudsky, G. Moghylny (p. #1.10). VSM magnetometer repair was done by E. Bersudsky. New software for VSM magnetometer control and data analysis is being created by I. Glavatskyy and E.Bersudsky. Maintenance and modernisation of the low-field magnetic susceptibility instrument was provided by E.Bersudsky and A. Dobrinsky. New equipment purchase (p.#1.10) was done by N.Glavatska, V.Gavriljuk (prepared the technical specifications and contract for mechanical testing machine), A.Urubkov, I.Glavatskyy (purchase of computers and accessories for cutting machine “MINITOM”), E.Bersudsky (temperature controller for X-ray diffractometer) and others.

Due to vacations and illness of G. Moghylny part of his planned the work on crystal structure investigation for melted alloys by X-ray diffraction methods was done by I. Glavatskyy and N. Glavatska by means of neutron diffraction (BENSC, HMI, Berlin) and I. Bojnitska (X-ray diffraction). Thus, it was necessary to redistribute the payment for the real amount of work been performed. It forced redistribution of the work planned for I. Bojnitska (furnace charge preparation and electropolishing of specimens) for V. Bliznjuk and A. Urubkov.

In addition, due to vacations and illness of A.Dobrinsky most part of his planed work on determination of phase transformation temperatures was done by A. Urubkov.

Since investigation of Ni-Mn-Ga compositions by X-ray fluorescent analysis method was performed at the first time, additional studies of etalon specimens of Ni, Mn & Ga and some methodology development was necessary. Thus, real amount of work performed for experimental investigation of electron structure was higher then it was planned. Funds for payment for I. Urubkov were partly transferred from those planned for G. Moghylny and A. Dobrinsky.

3. Description of travels.

Planned missions for the 1st quarter were cancelled. Funds for these missions were redirected for p. #7, Table 7, as it is clarified below (see Table Redirection).

4. Current status.

All activities were performed in accordance with project's work plan. Alloys with different Ni, Mn & Ga content were melted (p.#1.2). Started the investigation of the thermal treatment effect on the chemical alloy' composition (p.#1.2). Influence of the Ni, Mn & Ga concentrations on the phase transformation temperatures (p. #1.3) has been investigated. Four perspective compositions are chosen for further investigations. Optimisation of the single crystal growth technique is started (p.#1.4). Effect of the component concentrations on magnetisation (p.#1.5) and crystal lattice type (p.#1.6) of the selected perspective compositions is investigated. Performed the investigations of magnetic field induced deformation in selected compositions with higher martensite transformation temperatures (p.#1.7). Achieved etalon experimental spectra of the Ni, Mn & Ga electron structure and selected alloys (p.#1.8). Theoretical studies and modelling of the maximal and reversible deformations under simultaneous contrary applied magnetic field and compressive mechanical stress for the 5R martensite has been started (p.#1.9). Reconstruction and modernisation of the experimental equipment (goniometer of the 3-circle X-ray diffractometer, VSM magnetometer and low- field magnetic susceptibility instrument) was performed. Technical specification and construction for the device for automated control and temperature stabilisation for the high-temperature X-ray investigations (p.#1.10) is developed.

5. Problems encountered

As it was planned for the 1st quarter we purchased 6 computers including one for electron structure calculations, with total cost of $3711,3, paid for creation of temperature controller for X-ray diffractometer ($450,15),Diamond cutting wheels for STRUERS-MINITOM cutting mashine ($410,9), and purchased accessories for printer and copy machine ($40.71)

Due to summer vacations in ZAO EXITON ANALITIC firm, which is distributor of “Hounsfield Test Equipment Ltd' company, tender for mechanical testing machine manufacturers was delayed. After negotiations with “Hounsfield Test Equipment Ltd' company and its dealer ZAO EXITON ANALITIC in xUSSR countries, configuration and pricing was agreed. Contract for machine production was sent to “Hounsfield Test Equipment Ltd' company.

Purchase of 1st quarter planned equipment, namely: stabiliser CH ПТО ($355), power stabiliser for VSM magnetometer ($120) and one computer ($500) as well as chemical reactives (acids, ethanol etc - $20, argon - $20) and accessories ($10) was decided to delay until final agreement on configuration and pricing of primary cost equipment – above mentioned mechanical testing machine (Annex. 1, Table 4 #1).

Planned metals – Ni & Mn (Annex 1 Tabl 5 #2,3) were not purchased due to bad purity of proposed metals, according to performed chemical analysis data. Search for provider of pure metals in needed amount and purchase will be done in 2nd quarter.

We have bougth the diamond cutting wheels, which are planed to purchase in III Quarter (Annex1, Tabl. 4) inQuarter 1 because all our wheels for Cutting machine STRUERS “MINITOM” are fractured in August. These diamond cutting wheels are used for preparation of specimens according to the project work plan. As have shown our experiments in July and August, different compositions of the N-Mn-Ga alloys have different hardness and ductility therefore cutting of ingots with various alloys composition requires different types of wheels. Therefore we had to bay two types of wheels instead one type planned before. The price of wheels produced by STRUERS Company increased (254 EU) to compare with the planned ones ($160 Annex 1, Tabl. 4, p.17). We redirected cost for purchase of diamond wheels according to the Table given below: $121 is saved after purchase of the computers (Annex 1, Tabl.4, positions 2-7); $120 was planned for purchase of the Memory DIMM 32 Mb SDRAM for computer (Annex 1, Tabl.4, positions 11); $10 was planned for Communication (Internet, Phone, Post) (Annex 1, Table 7, p. 5).

We asked to redirect costs 1000 $ for travel by N. Glavatska, to Mexico, instead travels within Ukraine to Partenit Crimea, Sanct-Petersburg and Charkiv. Redirection costs are in the Table given below. N.Glavatska is invited for Plenary Lecture “Crystal structure and twinning crystallography in magnetic shape memory martensites of Ni-Mn-Ga” for SMCr Crystallography Congress, which will be held in the Mexican city Morelia (400 km from Mexico city) 9-14 November 2003 and also for lecture with the same topic for Mexican National Polytechnic Institute (Mexico) after the Congress. The SMCr Congress cancels the conference fee, pays for transportation from Mexico to Moreliya and back and for a Hotel (partially). Mexican National Polytechnic Institute will pay for fly tickets ($1200), accommodation in Mexico after the Congress ($350), terrestrial transportation ($55). Cost, which we ask additionally ($1000), is needed for a Visa ($100), daily money ($800) and additional money for the Hotel accommodation ($100). Details of redirection are given in the Table below.

Table. Redirection

Reference	New requested category,	Requeste	Original (old) category	Estimate	Redirecte

documents &date (1)	or old category with new cost (2)	d cost ((new) (3)	(4)	d cost (old) (5)	d cost (6) old – new
		Quarter <01>			
L01 27.08.03	1. Diamond Cuting disks Tabl.4, p.17	411	1. Diamond Cuting disks Tabl.4, p.17	160	+251
L01 27.08.03	2. Computers, Tabl. 4 p.2-7	3733	2. Computers, Tabl..4 p.2-7	3854	-121
L01 27.08.03	3. Communication (Internet, Phone, Post) (Annex 1, Table 7, p. 5.	0	3. Communication (Internet, Phone, Post) (Annex 1, Table 7, p. 5.	10	-10
L01 27.08.03	4. Memory DIMM 32 Mb SDRAM Annex 1, Tabl. 4, p11	0	4 .Memory DIMM 32 Mb SDRAM Winchester, Tabl.4,11	120	-120
Total by L01					411
L04 23.09.03	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	1000		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	0	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	700	-700
	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	0	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	120	-120
	4. Travel to Charkiv, Physical Technical Institute, Tabl.8 #3	-80	4. Travel to Charkiv, Physical Technical Institute, Tabl.8 #3	-180	-180
	Total by L04				1000

6. Delays and suggestions.

A part of equipment and materials planned for buying in 1 Quartal is not bought. We ask to permit to spend in 2 Quarter the costs saved in 1 Quarter on different sections, in accordance to the plan.

To optimize the works performance, to do the project management more operative, I ask for permission to redirect the planned work time for participants (6-8 days per month for one participant) and a type of work performed in between participants having the same qualification without preliminary agreement with EOARD and STCU. It is necessary due to some uncontemplated cases (for example: illness, business travels, a fracture of some equipment and so on).

N.Glavatska

Project Manager

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

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Financing parties: USA, European Office of Aerospace Research & Development (EOARD)

Reported period: 1 October 2003 - 31 December 2003
Date of the report submission: 8 January 2004

Content of quarterly progress report for Quarter 01

1. Summary of progress.

Stage number and title	1. Theoretical and experimental study of Ni, Mn, Ga contents influence on the phase transformations, electronic and crystal structure, magnetic properties and strain induced by the magnetic field
Actual progress	Study of Ni, Mn and Ga effect on temperatures of the phase transformation was continued in accordance with the task #1.2. Diagrams of the phase transformation temperatures dependence on Ni, Mn, Ga content are constructed using the referenced and our own results obtained due to the project performance. Results are directed on the main goal of the project the Ni-Mn-Ga composition optimization to produce high temperature magnetic shape memory alloys. Four polycrystalline ingots with weights 30g and 100g of the new off-stoichiometric compositions are melted (#1.2) basing on the results of 1 quarter. Single crystals were grown from three of these polycrystals with weight 30g (№ 68*, № N3) and 86 g (№ 25n) (#1.4). The temperature and velocity of the single crystal grown are studied and optimized. Different conditions of the single crystal growing cause difference in the Mn-content decrease, that affects difference in the chemical composition of the single crystals and results of difference in the phase transformation temperatures (#1.3) (Table 1).

Table 1. Chemical compositions and phase transformation temperatures

№	Ni, at%	Mn, at%	Ga, at%	M_S, ^{0}C	M_f, ^{0}C	A_s, ^{0}C	A_f, ^{0}C
68*	51.4	27	21.4	78	72	80	86
61*	50.3	28.3	21.4	40	41	42	47
N3	48,263	29,663	22,074	33	25	31	34
25n4 (middle of the single crystal)	46,743	32,151	21,106	57,5	50,50	55	65
25n2 (top of the single crystal)	46,543	32,445	21,013	126 76,9			

The composition's homogeneity was studied in the single crystals within a planes perpendicular to the crystallization direction and along this direction (st. #1.2). The big single crystal 25n (86 g) has some difference in the Ni, Mn and Ga content as before homogenization treatment as well as after it. That results in difference of crystal lattice type and the phase transformation temperatures (Table 1, Table 2). All studied single crystals have non-homogeneity in the Ni, Mn, Ga content after homogenisation and ordering treatments within planes perpendicular to the direction of crystallisation (Tabl. 2) (#1.2). That causes difference in the phase transformation temperatures and appearance of various types of martensite within the same plane (#1.2, #1.3, and #1.6). It is shown that the long time high temperature treatment, that is homogenisation, affects loosing of Mn from surface.

Table 2. Non-homogeneity of Ni, Mn and Ga content within plane perpendicular of the crystallisation axis in the 68* single crystal studied as results of the local chemical analysis.

Position	Ni, at%	Mn, at%	Ga, at%
A,Top Center	51.33	27.62	21.05
A, Top Outer	50.71	27.26	22.03
B, Bottom Center	49.81	27.93	22.26
B, Bottom Outer	51.58	27.48	20.94

Study of the structure of the bulk specimen of the same single crystal using neutron diffraction (BENSC, HMI Berlin) shows that the main part of the crystal has the orthorhombic 7-layered modulated structure of martensite; however 5-layered modulated martensitic structure also is observed (#1.6). The martensite structure of the thin specimen, which was cut out from the central part of the 68* sample, is studied using the transmission microscopy analysis at room temperature. It is found that the main part of the specimen has orthorhombic 7-layered modulated structure of martensite, however, there are some areas having non-modulated tetragonal *bct* martensitic structure (#1.6).

The long time exposure at the high temperature during the homogenisation treatment causes appearance of areas with the stoichiometric composition, that is energetic preferable, and as result, existence of some areas having decrease/ rise in Ni, Mn and Ga content (##1.2, 1.3, 1.6). That causes difference in the martensite crystal structure as in bulk crystal, as well as within small areas of it. As result it effects properties (including of the magnetic file induced strain) of single crystals. These results show importance of treatments correction that will be continued during the 3 quarter.

The temperature dependence of lattice parameters for 7-layered modulated structure of martensite of 68* single crystal is studied from start of martensite transformation temperature (78^{0}C) until room temperature (#1.6). Temperature dependence of magnetization in the same crystal also is studied within temperature range from (80^{0}C) down to minus 73^{0}C (#1.7). According to that study the 7-layered modulated structure of martensite exists until this temperature and no another martensitic transformations are occurred (#1.5, 1.6).

Energies of the phase transformations (austenitic, martensitic and magnetic) are calculated by using the experimental data for crystals with different types of the martensitic structures (7M, 5M and *bct*-nonmodulated) (#1.3). The composition of the alloy with 7M modulated structure has the biggest enthalpy and entropy change for both types of transformations (Table 3) (#1.3).

Table 3. Enthalpy and entropy for the martensitic and magnetic transformation in Ni-Mn-Ga crystals

№	Austenite, J/g	As, C	dS, /gK	Curie point, J/g	Tc, C	dS, J/gK	Structure
61*	-4,24	41	-0,103	-0,125	101	-0,001238	5M
68*	-9,64	80	-0,12	-0,225	104	-0,002163	7M
C	-8,765	168	-0,052	-0,055	110	-0,0005	*вст,* non-modulated

Alloy „C" (Ni52.4Mn25.6.2Ga22)

In accordance with the magnetization study, all mentioned above crystals (Tables 1-3) have a strong magnetic anisotropy (#1.5). The single crystal “C” with the bct non-modulated structure has a plane of easy magnetisation. The temperature dependence of magnetisation is studied within temperature range from the start martensite transformation temperature down to 200K for crystals with 7M and 5M modulated structures (#1.5).

Mobility of twins results of appearance of magnetic shape memory, in the other hand, the mobility of twins can dependent on twin’s crystallography, therefore an effect of cooling conditions during martensite transformation on twinning and on the twins crystallography is studied for 5M martensite structure (#1.6, as some special part of the treatments effect study. It is shown that elastic-inelastic twin’s structure having a lot of the stacking faults is formed due to the free cooling at air. This structure is stable and does not relax with time (#1.6). If the specimen is cooled under magnetic field with the same rate down to room temperature, the twin structure having much more mobile boundaries is formed. The staking faults relax with time (#1.6). Study an effect of the cooling conditions on twinning will be continued during the 3 quarter.

Effect of cooling conditions, magnetic and mechanical cycling on magnetic field induced strain is studied as for 5M martensite showing giant magnetic field induced strain (alloys Ni49.7Mn28.7Ga21.6, 61*, N3 (Table 1), as well as for *bct* martensite structure (crystal “C” Ni52.4Mn25.6.2Ga22) (#1.7). The velocity of the dynamic response of the martensitic structure on the magnetic field also studied by experimental and theoretical methods (#1.7, #1.9). That is important to obtain the maximal velocity of the magnetic field induced strain in the magnetic actuators and to understand, which factors control this process. These experimental results are some basis for a theory of the dynamic response velocity, which development is started (#1.9).

Development of a theory of the micro-twin’s martensite started. We have found some formulas for the lattice parameters calculation for multilayered martensite, basing on fct martensite with (c/a>1) (#1.6). This kind of presentation of the Ni-Mn-Ga martensite structure gives some possibility to explain all known types of martensite as some polytypic modification a tetragonal martensite. Also, that can explain an important experimental fact: the martensite tetragonality ratio c/a decreases with the temperature rise.

The electronic structure of the alloy 61* is studied by using a complex of experimental and theoretical methods (#1.1, #1.8). The experimental X-ray fluorescent emission spectres were obtained as for austenite with fcc crystal lattice, as well as for martensite with 5M modulated structure (#1.8). Interpretation of experimental data was carried out by comparison with results of electron band structure calculation. The off-stoichiometry was ignored in the theoretical modulation; the real 5M lattice was approximated by the bct unit cell (#1.1). The spin-polarized variant of the LAPW – method and the structure date were used for the total -and partial density calculation. The LSDA - local spin density approximation was used for the theoretical band-structure calculation. Comparison of the experimental spectra with the calculation result was made using the main maximums. The total- and partial- spin densities for fcc and bct phases in 61* alloy (Tabl.1) were studied by using this complex method. It is found (sub-stage # 1.8, #1.1) in the 61*alloy:

-the Ni3d electrons dominate on the Fermi level;

- the valence electrons band contents two parts: (a) near-Fermi level is located at about of ~ 10 eV for the fcc cell, and ~ 7 eV for the bct martensite, which is formed preferable by hybridized Ni and Mn ; (b) a thin band with the energy at about 14 eV, that is formed by the 3d electrons of Ga;

- There is strong interaction between Ni and Mn atoms, the interaction of the Ga- atoms with the another ones is poor;

- The magnetic moment of Mn and Ni atoms rises due to austenite-martensite transformation: on 0.76Ev for Mn and 0.35Ev for Ni. That causes rise of the magnetic moments of unit cell (+1.52 Born magneton) (Table 4).

Table 4. Magnetic moments of austenite and martensite unit cells of the 61* alloy Ni-Mn-Ga

fcc (austenite)			bct (martensite)	
Atom	Magnetic moment, E_v		Atom	Magnetic moment, E_v
Mn	3.45807		Mn	4.22192
Ni	0.35622		Ni	0.70911
Ga	-0.04884		Ga	-0.03453
Unit cell	4.13088		Unit cell	5.65017

2. Summary of personnel commitment.

The program of study within sub-stage #1.2 is performed by the participants of the project: N.Glavatska, V.Gavriljuk (searching for the alloy composition and conditions of heat treatments), I.Glavatskyy (local chemical analysis and calculation of enthalpies and entropy change of the phase transformations), A.Urubkov and V. Bliznjuk (melting of polycrystals), E.Tarusin (heat treatments and preparation of some specimens), I. Surzhenko (Bojnitska) (orientation of single crystals by X-ray texture methods). A.Urubkov studied effect of the magnetic and mechanical cycling on phase transformation temperatures. Chemical analysis of single and polycrystals was done also by V.Burtzev, who does not participate in the project.

I. Urubkov, A.Urubkov and V.Uvarov have studied the electron structure (sub-stages #1.1 and #1.8) I.Urubkov has studied the electron structure of alloy 61* in austenitic and martensitic phases with experimental methods using the X-ray fluorescent emission spectrometer (sub-stage #1.8). A.Urubkov studied an electronic structure in austenite and martensite for the same alloy using modelling method using WIEN-2K program (#1.1, #1.1). V.Uvarov has calculated electron structure based on experimental spectra and results of modelling of electronic structure of austenite and martensite in 61* alloy (sub-stages #1.1, #1.8).

Study within #1.3 sub-stage tasks was done by I.Glavatskyy (measurement of the phase transformation temperatures by DSC method and tensometry), A.Dobrinskiy (measurement of the magnetic transformation temperatures with the magnetic susceptibility method). I.Zasimchuk and L.Matvienko studied effect of the single crystal grown conditions on quality of single crystals with goal to improve it and have grown single crystals (sub-stage #1.4). Magnetisation and its temperature dependence in single crystals 68*, 61* were studied by I.Glavatskyy (sub-stage #1.5).

Crystal structure of austenite and martensite in the alloy 61* was studied with neutron diffraction by G.Mogilnyy (#1.6). I.Glavatskyy has studied the crystal structure and temperature dependence of the martensite lattice parameters by neutron diffraction in 68* single crystal (#1.6). V.Bliznjuk studied structure of martensite in 68* sample by transmission electron microscopy (#1.6). Twinning crystallography is studied by G.Mogilnyy with X-ray diffraction methods (#1.6). He studied also together with A.Dobrinskiy the effect of cooling conditions on twinning (#1.6). Magnetic field induced strain (#1.7) was measured by O.Rudenko and I.Glavatskyy. V.Lvov (theoretically) A.Rudenko (modelling and experiment) and I.Glavatskyy (experiment) studied rate of dynamic response of the martensite structure on magnetic field action. (st. #1.9).

A working model of temperature controller for X-ray diffraction study at high-temperatures is made. E. Bersudskiy corrected the computer's program and optimised of parameters of mentioned equipment (#1.10). Some repair of the magnetic dilatometer and correction of computer program for it is made (managed by V.Cherepin) (#1.10). A.Marunjak and O.Rasumov constructed and made some mechanical devices for *maintenance of X-ray* texture goniometer and heating device. Both of them are not participant of the project. M.Knysh made some prophylactic and partial repair of the water cooling system for dilatometer. He also made some locksmith works (#1.10). N.Glavatska managed and planed all scientific studies and works within sub stages #1.1-#1.10, corrected tasks, interpreted results obtained, have written reports.

3. Description of travels.

N.Glavatska has travel to Mexico, participating with the plenary lecture "Crystal structure and twinning in the magnetic shape memory martensites of Ni-Mn-Ga" in SMCr-2003 Crystallographic Congress (Mexico, Morelia city) and has given lecture for that theme for Mexican National technology Institute (Mexico city).

4. Current status.

Activities were performed in accordance with project's work plan. Poly crystals and single crystals with different Ni, Mn and Ga content were melted and grown (#1.2, #1.4). Influence of the Ni, Mn and Ga content on the phase transformation temperatures (#1.3) is continued. An effect of the thermal treatment on the alloy composition as well as on the phase transformation is studied (p.#1.2).. Optimisation of the single crystal growth technique is made Three single crystals are grown (p.#1.4). Magnetisation and its temperature dependence in searched alloys is studied (#1.5). Crystal structure of martensite for selected alloys compositions and temperature dependence of lattice parameters for single crystal with high temperature of martensite transformation (~78^{0}C) is studied (#1.6). Investigation of an effect of cooling conditions on twinning is started (#1.6). The magnetic field induced strain was studied in the new selected crystals Investigation of rate of dynamic response of the martensitic structure to the magnetic field action is started (#1.7, #1.9). Electron structure in austenite and martensite in the alloy displaying giant magnetic field induced strain is studied using experimental and theoretical methods (#1.8, #1.1). Reconstruction and modernisation of the experimental equipment (goniometer of the 3-circle X-ray diffractometer, heating device, temperature controller for diffractometer) was performed. (st.#1.10).

5. Problems encountered

According to the Project agreement it is paid an advance ($7373.6) for purchase of the mechanical testing machine produced by "Hounsfield Test Equipment Ltd (Annex 1 Table 4 #1). The diamond cutting discs STRUERS are bought for cutting machine MINITOM STRUERS according to the Project agreement Annex 1 Table 4 #17). A performance of power supply for temperature controller for X-ray diffractometer is started and bought partially (Annex 1 Table 4 #20). Some special device and holder for the high temperature x-ray study is constructed and paid (Annex 1 Table 7 #2). Some pure metals: Ni (500g), Mn (500g) and Ga (150g) were bought not with the project costs. Costs redirection occurred during the 2Qv are explained in the table below.

Table. Redirection 2Qv.

Reference documents &date (1)	*New requested category,* or old category with new cost (2)	Requested cost (new) $ (3)	*Original (old) category (4)*	*Estimated cost (old)* (5)	Redirected cost (6) $ *old – new*
L03 227.08.03	1. N.Glavatska (Payment by cash for power supply temperature controller according the project agreement) Tabl.3, p.1	100			+100
	2. Power supply for temperature controller, Tabl. 7, p 20	0	2. Power supply for temperature controller, Table 7, p 20	100	-100
L01 27.08.03	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder), Tabl.3, p.1	150			+150
	2. Repairing/maintenance of equipment Tabl.7, p 6	0	2. Repairing/maintenance of equipment Tabl.7, p 6	150	-150
	Total 2 Qv				$250

6. Delays and suggestions.

A part of planned materials and equipment was not purchased. We have to save money for much more important devices needed to provide the project study. I ask for permission to spend a part of costs saved during 1-2 Qv on different sections for purchasing of the digital photo camera, an optical device and optical converter for the Karl ZEISS microscope in 3Qv. We need these devices extremely. We have bought some digital photo camera before this Project started (in April 2003), therefore purchase of mentioned devices was not planned. However, the optical devices needed for connection of our new digital camera and with the quite old type Karl ZEISS microscope are not produced in the present time. Therefore, we have to buy the digital photo-system mentioned above in the complex to provide the microscopic structure study and the magnetic domain structure investigation.

N.Glavatska

Project Manager

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

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Institutions: Institute for Metal Physics
Financing parties: USA, European Office of Aerospace Research & Development (EOARD)
Operative commencement date: 1 January 2004 - 31 March 2004
Project duration: 2 years
Date of submission: 9 March 2004

	Content of the quarterly progress report for quarter <03>	PAGE 1

1. Summary of progress.

Stage number and title	#1. Theoretical and experimental study of Ni, Mn, Ga contents influence on the phase transformations, electronic and crystal structure, magnetic properties and strain induced by the magnetic field

Actual progress The perspective compositions Ni-Mn-Ga having higher temperatures of martensitic transformations are selected basing on results of 2Qv. The polycrystalline specimens are melted, homogenized and ordered Effect of difference
in the heat treatment (re-melting and homogenization) is studied (#1.2). Result of the chemical analysis of new melted alloys is given in the Tabl.1

Table 1. Chemical compositions and phase transformation temperatures for poly- and single crystals

№	Name	at%			^0C				
		Ni	Mn	Ga	Tc	M_S	M_f,	A_s	A_f,
1	**25n_z4 (single crystal)**	**46,8***	**32,2***	**21,1***	**85,8**	**59,5**	**50**	**59,7**	**69**
2	**25n_z1 (single crystal)**	**45,50**	**33,87**	**20,62**	**85,9**	**57,5**	**50,5**	**51,6**	*
3	**A68-I (polycr)**	45,50	33,87	20,63	**87,5**	**83**	**68**	**72**	**87**
4	**68V-n (polycr.)**	*	*	*	**87**	**60**	**58**	**65**	**67**
5	68-F-V (polycr.)	49,3	28,9	20,9	87,5	40,7	39	49	61
6	BV-68 (polycr.)	47,9	26,1	25,8	87	39,1	38,4	51,7	52,1

*- will be corrected

Single crystals were grown from 3 perspective polycrystals having higher temperatures of the martensitic transformations temperatures (#1.4) Effect of cooling ratio on quality of single crystals is studied. An effect of change in the chemical composition on the phase transformation temperatures for new melted single crystals is studied (Tabl.1) (#1.3). It is shown that rise in the Mn content instead of Ni and Ga causes increase of the martensitic transformation temperature (Tabl.1) and some decrease of the ferromagnetic transformation temperature. Almost all melted and studied in 3 Qv alloys have the big martensite tetragonality (#1.6) (that determines value of the magnetic field induced strain) and strong magnetic anisotropy (#1.5). Crystals having the higher martensitic transformation temperatures, small temperature hysteresis of phase transformations, strong magnetic anisotropy and big tetragonality ratio (are marked with bold in the Tabl.1), are selected for following study of magneto-plastic behavior. Within the stage (# 1.4) a method for study of multilayered structures and they're details using 3- circle diffractometer is developed. That is important for correct determination of the crystal lattice in thestudied Heusler alloys.

Basing on statistical theory of magneto-plasticity, developed by authors of the project early in year 2003, the time- dependent behavior of the magnetic field induced strain is studied using both- theoretically and experimental methods (#1.9б, #1.7). The theory of time-dependent stability of the dynamical response of ferromagnetic martensities to the constant magnetic field action is proposed. The article "Time-dependent magnetostrain effect in ferromagnetic martensite: Theory and experiment "by V. L'vov, O.Rudenko, N.Glavatska is submitted for publication in the Physical Review B (the copy of the article is attached.

The space group of crystal lattice for composition of Ni-Mn-Ga displaying giant magnetic shape memory is identified by using theory of groups. It is important for correct calculation and modeling of the electronic structure. The space group for the 5 layered martensite Ni-Mn-Ga is determined as P2/m (№10 according to the International tables). Unit cell of this lattice has 40 atoms. The coordinates of non-equivalent atoms are determined (#1.1). Calculation of the electronic structure (band calculation) is made for *bct* approximation of the real 5- layered structure for stoichiometric approach at 300K. Also electronic structure is calculated fro real *bct*- cell at temperatures 300K and 450K within the stoichiometric approximation. Graphics of full and partial densities are done (# #1.1, 1.8). An article is being written.

Maintenance and modernization of magnetometer, magnetic dilatometer is continued as well as optimization and making of the mechanical device for high temperature system for x-ray diffractometer (#1.10).

#2. Preliminary study an effect of alloying elements on the phase transformation and structure

Effect of alloying of the Ni-Mn-Ga compounds by Fe on the phase transformation temperatures is studied in accordance with plane of the Stage 2. Seven polycrystalline ingots with different Fe content were melted (Tabl.2). Samples for studies were prepared after heat treatment of the ingots (#2.1).

The phase transformations in new Ni-Mn-Ga-Fe alloys were studied using low field magnetic susceptibility and tensometry methods (#2.2). It is shown tendency in rise of the temperature magnetic transformation T_c with the Fe contend rise (Tabl.2). Some tendency of decrease in the martensitic transformation temperatures is also observed, however, this conclusion should be confirmed basing on higher statistics of experimental results. This preliminary study shows, that rise in Ni- content in Fe- alloyed specimens (when Fe is added instead of Mn) causes rise of the martensitic transformation temperatures (Tabl.2). Temperature of martensitic transformations is lower then the magnetic transformation temperature in all selected compositions of the Ni-Mn-Ga-Fe alloys. Alloy № 4 seems to be very perspective for followed study because the martensitic phase exists from 108,2^{0}C down to minus 50^{0}C. All another compositions have the martensite transformation temperatures lower then Curie temperature and austenite exists down to low temperatures (Tabl.2).

In accordance with x-ray diffraction data (#2.4), alloy №3 has the tetragonal lattice of martensitic phase at room temperature with the lattice parameters c=6.64 A, a=b= 5.40^{o}A. The martensite tetragonal ratio is in this alloy very big: (1-c/a) = 22.9%. The austenite lattice parameters for №№ 2, 4, 5 alloys are almost equal at room temperature: a=b=c= 5.81^{o}A.

Alloy № 2 with Fe (table 2) possesses strong magnetic anisotropy, high martensite tetragonality ratio together with high martensite phase transformation temperatures making it perspective for further studies of crystal structure and magneto-plastic properties.

Table 2. Chemical composition and phase transformation temperatures

			at%					^{0}C		
№	**#**	**Ni**	**Mn**	**Ga**	**Fe**	T_c	M_S	M_f,	A_s	A_f
1	Se17'03**	46,8	26,54	25,7	0,71	99,5	-13	-33	-28	-13
2	F12'04c1	46,96	22,89	24,88	5,27	106	-83,4	-119	-117	-93
3	**F12'04b1**	**52,15**	**16,96**	**21,26**	**9,63**	**115,5**	**108,2**	**96,6**	**99,9**	**115**
4	F12'04d1	45,85	20,32	24,05	9,78	157	*	*	*	-153,4
5	Feb27'04b	49,57	16,05	20,74	13,64	149	0.5	-61	-49,7	8,4
6	Oc23d	49,97	18,68	20,43	10,92	165	-84,8	-63,4	-79,3	-56
7	Oc23c	49,95	9,44	25,95	14,66	166,6	-64,8	-88,5	-88,5	-64,8

* - requires re-determination, **- Si -1,00%, Al-0,29%

2. Summary of personnel commitment.

Electron structure studies (sub stage #1.1 & 1.8) were performed by I. Urubkov (experimental studies of *bct*-alloy in austenite and martensite phase) (#1.8), V. Uvarov (computation and modeling of experimental spectra) and A. Urubkov (mathematic modeling) (#1.1). In sub-stage #1.2 & 2.1 were involved: N. Glavatska, V. Gavriljuk (choice of compositions, polycrystals melting and annealing routine), A. Urubkov, V. Bliznjuk (melting, specimen preparation), E.Tarusin (annealing), I.Surzhenko /Bojnitska (the orientation analysis of poly- and single-crystalline specimens by X-ray texture analysis). Chemical analysis was performed by V.Burtsev, not a project participant. Tasks #1.3 is performed by I.Glavatskyy (determination of phase transformation temperatures by DSC and dilatometry). Single crystals (#1.4) were grown by I.Zasimchuk and L.Matvienko. Magnetisation (#1.5) was studied by I. Glavatskyy. G.Moghylnyy performed investigations of crystal structure of austenite and martensite phases (#1.6, 2.4). N.Glavatska and G.Moghylnyy have developed X-ray technique for modulated (multilayer) structure investigation (#1.6, 2.5). Magnetic field induced strains (#1.7) were studied by O.Rudenko and I.Glavatskyy. Theoretical modeling and investigation of dynamic response velocity on magnetic field (#1.9) were performed by V.Lvov (theoretical approach), O.Rudenko (mathematic modeling, experiment), I.Glavatskyy (experiment, theoretic approach). A. Dobrinsky investigated influence of Fe alloying on phase transformation temperatures (#2.2) by means of low-field magnetic susceptibility and dilatometry. E.Bersudskiy was developing special equipment for temperature controllable specimen holder for X-ray diffractometer and magnetometer renewal (together with I.Glavatskyy) (#1.10). Renewal and upgrade of dilatometer´ temperature controller was performed by #1.10 (responsible – V.Cherepin). We also invited A. Marunjak and M. Kovalik (both not a project participants) for design, engineering and manufacture of precise mechanical spare-parts and devices for X-ray diffractometer temperature control system. M.Knysh performed technical maintenance of furnace´ vacuum system as well as some required metalwork’s and locksmithing. N.Glavatska performed scientific guidance, management, results interpretation and co-ordination by all project stages (#1.1-1.10, 2.1-2.4). Due to G.Moghylnyy disease his job was partially redirected to A.Dobrinsky.

3. Description of travels.

N.Glavatska participated in “Interplay of Magnetism and Structure in Functional Materials” workshop held 9-14 February 2003 in Benasque (Spain) with the talk “Magnetic creep in the magnetic shape memory Ni-Mn-Ga in the steady magnetic field”.

4. Current status.

Scheduled tasks were performed according to project work-plan. By stage 1 were produced Ni-Mn-Ga poly- and single- crystals with higher martensite transformation temperatures (##1.2-1.4). Magnetization of single crystals was investigated (#1.5). Crystal structures of perspective compositions of poly- and single- crystals were investigated. We developed the technique for modulated (multilayer) crystal structure investigation by means of 3-circle X-ray texture diffractometer (#1.6). Magnetic field induced strain and dynamic response of crystal structure on different magnitudes of applied field (#1.7, 1.9) in chosen crystals was investigated. Theory of time-dependent magnetic field induced strain has been developed. Theoretically and experimentally investigated electron subsystem, density of states in Ni-Mn-Ga crystals with *fcc* and *bcc* lattice (#1.8, 1.1) in austenite and martensite states (#1.8).

By stage 2 ingots of Ni-Mn-Ga-Fe alloys with different Fe content are prepared. We have investigated effect of Fe- alloying on phase transformation temperatures and phase-structural state (##2.1-2.4).
Automated temperature control system for high-temperature X-ray studies is been developed and tested (#1.10).

Activities were performed in accordance with the project work plan. Poly crystals and single crystals with different Ni, Mn and Ga content were melted and grown (#1.2, #1.4). Influence of the Ni, Mn and Ga content on the phase transformation temperatures (#1.3) is continued. An effect of the thermal treatment on the alloy composition as well as on the phase transformation is studied (##1.2).. Optimisation of the single crystal growth technique is made Three single crystals are grown (##1.4). Magnetisation and its temperature dependence in searched alloys is studied (#1.5). Crystal structure of martensite for selected alloys compositions and temperature dependence of lattice parameters for single crystal with high temperature of martensite transformation (~78^{0}C) is studied (#1.6). Investigation of an effect of cooling conditions on twinning is started (#1.6). The magnetic field induced strain was studied in the new selected crystals Investigation of rate of dynamic response of the martensitic structure to the magnetic field action is started (#1.7, #1.9). Electron structure in austenite and martensite in the alloy displaying giant magnetic field induced strain is studied using experimental and theoretical methods (#1.8, #1.1). Reconstruction and modernisation of the experimental equipment (goniometer of the 3-circle X-ray diffractometer, heating device, temperature controller for diffractometer) was performed. (st.#1.10).

5. Problems encountered

Mechanical-testing machine “Hounsfield Test Equipment Ltd” was purchased, as it was planned (Annex 1, Table 4, #1). We purchased optical adaptor for digital photocamera and optical microscope Carl Zeiss “Ergaval”. Also we purchased office and spare-materials for Xerox copier and printers. For mission of N.Glavatska to Benasque (Spain) for “Interplay of Magnetism and Structure in Functional Materials” workshop we used $306 transfer additionally to money planned by project (letter L06). It was necessary to cover expenses due to flights mismatch with seminar opening and closing dates. According to letter L07 $582 was transferred for purchase from Ibendorf & Co Ingenieur- und Vertriebs GmbH of optical adaptor to equip our Carl Zeiss microscope with digital photo camera. According with letter L08, $120 paid cash for chemical analysis of new alloys and manufacturing of needed spare-parts and equipment repair (dilatometer and magnetometer). $100 transferred for cash payment (L08) for manufacture of special thermo-controllable specimen holder for X-ray diffractometer (as planned in Annex 1, Table 7, #2) and special chemical-mechanical method of the specimen preparation. Details are explained in table below:

Table. Redirection 1 Qv.

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)
Redirection 1 Qv					
L01 27.08.03	1. Diamond Cuting disks Tabl.4, #.17	411	1. Diamond Cuting disks Tabl.4, #.17	160	+251
	4. Memory DIMM 32 Mb SDRAM. Annex 1, Tabl. 4, #	0	4 .Memory DIMM 32 Mb SDRAM. Winchester, Tabl.4, #11	120	-120
L04 23.09.03	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	1000		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	0	2. Travel to Partenit Crimea for ISFD conference, Tabl.8, 1	700	-700
	3. Travel to Sankt-Petersburg, Russia, Tabl.8 #2	0	3. Travel to Sankt-Petersburg, Russia, Tabl.8 #2	120	-120
	4. Travel to Charkiv, Physical - Technical Institute, Tabl.8 #3	80	4. Travel to Charkiv, Physical - Technical Institute, Tabl.8 #3	180	-180
	Total by 1Qv				1411
Redirection 2Qv					
L02 27.08.03	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder according to the project) Tabl.3, #.1.	150			+150
	2. Repairing/maintenance of equipment Tabl.7, # 6	0	2. Repairing/maintenance of equipment Tabl.7, # 6	150	-150
L03 27.08.03	1. N.Glavatska (Payment by cash for power supply temperature controller, Tabl.3, #.1	100			+100
	2. Power supply , Tabl. 7, # 20	0	2. Power supply for temperature controller Tabl. 7, # 20	100	-100
	2. Repairing/maintenance of equipment #6 Table 7	84	Repairing/maintenance of equipment #6 Table 7	150	-66
	Total 2 Qv				$316
Redirection 3 Qv					
L06 23.09.03	1. Workshop “Interplay of Magnetism and Structure in Functional Materials” in Benasque (Spain), #3, Tabl.8,	1506	1. Workshop “Interplay of Magnetism and Structure in Functional Materials” in Benasque (Spain), #3, Tabl.8,	1200	+306
	2. Travel to Berlin, Germany 2Qv #2,Tabl.8	0	2. Travel to Berlin, Germany, #2Tabl.	220	-220
	3. Repairing/maintenance of	64	3. Repairing/maintenance of	150	-86

	equipment (1Qv) #6,Tabl.7		equipment (1Qv) #6,Tabl.7		
	Total L06				306
L07 19.02.04	1. Adapter and Step down ring for optical microskope #21, Tabl.4	582	1. Adapter and Step down ring for the optical microskope #21, Tabl.4	0	+582
	2. Stabilisator of voltage #14, Tabl. 4	0	2. Stabilisator of voltage #14, Tabl. 4	355	-355
	3. Communication (1-3Qv) #5,Tabl.7	0	3. Communication (1-3Qv) #5,Tabl.7	55	-55
	4. Chemical analysis (1Qv),#5,Tabl.7	0	4. Chemical analysis composition, (1Qv),#5,Tabl.	30	-30
	5.Computers (1Qv) ,##2-7,Tabl.4	3354	5.Computers (1Qv) ,##2-7,Tabl.4	3212	-142
	Total by L07				582
L08 23.02.04	1. N.Glavatska Tabl.3, #1	120	1. N.Glavatska Tabl.3, #1		+120
	2. Chemical analysis, Tabl. 7, # 11	0	2. Chemical analysis, Tabl.7, # 11	30	-30
L08 23.02.02	3. Repairing/maintenance of equipment, Tabl.7,#8	60	3. Repairing/maintenance of an equipment, Tabl.7, #8	150	-90
	Total by L08				120
L09 1.03.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L09 16.03.04	2. Special holder and divice for diffractometer Tabl. 7, # 2	0	2. Special holder and divice for diffractometer, Tabl. 7, # 2		-100
	Total by L09				100
	Total 3Qv				1108

6. Delays and suggestions.

Due to defective power supply system by Institute for Metal Physics to VSM magnetometer laboratory room 143, magnetometer unit was broken again. Thus instrument requires significant repair which could cause troubles (delay) in project stage #2.3.

I ask for your permission to use in 4rd quarter costs been saved in 1st-3nd quarters for purchase of necessary equipment – the defect-free chemical crystal cutting and polishing machines and office copier.

N.Glavatska

Project Manager

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

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Financing parties: USA, European Office of Aerospace Research & Development (EOARD)
Operative commencement date: 1 January 2004 - 31 March 2004
Project duration: 2 years
Date of submission: 12 June 2004

Content of the quarterly progress report for quarter <04> PAGE 1

1. Summary of progress.

Stage number and title	***#2.Preliminary study an effect of on alloying elements the phase transformation and structure***
Actual progress	Study of the alloying effect on the phase transformation temperatures of Ni-Mn-Ga is continued. New compositions of Fe-alloyed Ni-Mn-Ga were melted basing on the results obtained in previous quarter concerned the effect of Fe on the martensite transformation temperatures. Fe was added instead of Mn and Ga in new alloys (# 2.1). Polycrystals with different Fe-content were made using two- or four- step remelting followed by homogenization and ordering treatments. Chemical analysis of new alloys was done. Phase transformation temperatures of new melted alloys were determined (## 2.1, 2.2, 2.3). We have studied the effect of alloying by other elements (Sn, B, Si) on the phase transformation temperatures Ni-Mn-Ga, as well as effect of complete substitution of Ga and Mn with Sn and Fe correspondingly. Chemical compositions and temperatures of the phase transformation are presented in Table 1.

Table 1. Chemical composition and phase transformation temperatures.

	at%				^{0}C				
Name	**Ni**	**Mn**	**Ga**	**Fe**	**Tc**	**M_S**	**M_f,**	**A_s**	**A_f**
N25-2	51,81	23,28	24,2	0,71	102	29	11	21	31
AF1	53,5	-	26,5	20	*	47	32	*	*
ApF2	49,42	27,62	21,34	1,79	113	43	55	54	59
	Ni	**Mn**	**Ga**	**Sn**					
MSn1	50,51	25,09	0	24,40	73	-	-	-	-
MSn2	42,5	32,5	0	25	89	-	-	-	-
MSn3	49,0	29,5	10,5	11,0	85	*	*	*	*
MSn4	49	26	22	3	106	*	*	*	*
	Ni	**Mn**	**Ga**	**B**					
MB1	50	25	0	25	75	-	-	-	-

JB2	60	20	0	20	80	-150		-120	
	Ni	**Mn**	**Ga**	**Si**					
JSi1	48,2	30,8	18	3	109	-	-	-	-

* - requires re-determination,

All melted alloys are strongly ferromagnetic (#2.3). New alloys with Fe have martensite at room temperature: N25 – orthorhombic with 5-layered modulation, ApF2- mixed 5- and 7-layered, Af1- tetragonal non-modulated (#2.4). Alloy NAF-J2 has martensitic and magnetic transformation within the temperature interval (200-10,6^{0}C), the inter-martensitic transformation occurs with cooling (Tabl.1). Alloying by Sn, Si and B decreases the transformation temperatures for chosen concentrations of Ni-Mn-Ga. Alloying by small quantity of Fe for single crystal N25a slightly decreases martensite transformation temperatures and lattice parameters but does not affect its magneto-mechanical behavior. The magnitude of the MFIS (2-4,5%), as well as the critical field value needed for twin boundary activation at room temperature is practically the same, as for basic Ni-Mn-Ga compositions (#2.5). Experimental and theoretical study of electronic structure of the ApF2 and F12'04b1 crystals alloyed by Fe, melted in the previous quarter, is started (# 2.6, 3.5).
Analysis of the alloying effect by Fe on the phase transformation temperatures in Ni-Mn-Ga is done< basing on present results as well on the results obtained during 2nd and 3rd quarters. The referenced published results were also taken into account. Dependences of the Curie point and austenite transformation temperatures on Fe-content are constructed. Effect of alloying on changes in electron concentration and its effect of transformation temperatures are analyzed as well. It is shown that alloying by Fe causes rise of magnetic transformation temperature, which can be approximate by linear dependence:

$$T_c = 95{,}092 + 4{,}103 * Fe(at\%).$$

Rise of the Curie temperature, due to decrease of the unit cell volume, is caused by Fe alloying. Effect of Fe on the martensitic transformation temperatures is complicated and depends on element that is substituted Ni, Mn or Ga and requires building the set of 3-dimensional phase diagrams. <u>An article concerned the alloying by Fe on transformation temperatures in Ni-Mn-Ga is prepared for publication.</u>

#3 Optimization of compositions. Study of the constitution of the alloys having high temperatures of ure transformations

Polycrystals with corrected compositions were melted. Single crystals were grown from perspective polycrystals, having higher transformation temperatures and important for following fundamental studies (##3.1-3.3). Temperatures of phase transformations are determined and presented in Tabl.2. Crystal structure of new single crystals is studied (#3.6).

Table 2. Chemical composition, transformation temperatures and crystal structure

	at%				^{0}C					Structure
Name	**Ni**	**Mn**	**Ga**	**Fe**	**Tc**	**M_S**	**M_f,**	**A_s**	**A_f**	
N5_A5 Single crystal	47,34	25,86	20,38	6,42	114	94	82	104	114*	5M
JF_25	50.05	28.04	20.22	1.69	101*	51	43	53	60	5M
N25_A25 Single crystal	48,83	28,76	22,32	0,08	100	33	31	38	40	5M
BG66 Big grain	53,9	24,4	21,7	-	106*	168 66	159 62	180 71	183 80	bct, orthorhombic
1A	48,54	27,12	24,34		102	>210	-	-	-	Monoclinic
Ap9F (single crystal)	49.94	21.89	20.95	7,23	118	96	90	108	112*	Tetragonal

* - requires re-determination,

Details of crystal structure in some single crystals grown in previous quarters are studied using neutron diffraction (68b_z, A1), transmission electron microscopy (68B) and x-ray diffraction (66B, 25N, BG66, N3, F12'04b1) (#3.6). Martensite in single crystal 68B consists of mixed structure: tetragonal non-modulated, 5M- and 7M modulated. Alloy BG66 has tetragonal non-modulated thermal martensite. Due to the applied magneto-thermo-mechanical treatment a stress-induced martensite with orthorhombic modulated structure was induced in the single crystal BG66. This martensite structure remains stable even above 55^{0}C, after applied stress was taken off. Difference in ***a*** and ***c*** lattice parameters in this martensite is

23% at 52^0C. Reorientation of martensitic variants under magnetic field at room temperature and at 52^0C is studied in-situ with x-ray diffraction. Observed reorientation of martensitic twin variants at 52^0C corresponds to the magnetic field induced strain of 11,6%. We are preparing an article for publication basing on this result obtained. Magnetic properties high-temperature alloys are studied. Single crystal BG66 possesses unordinary magnetization behaviour and shows very strong and unique angular dependence of magnetization (#3.4). Mechanical properties of crystals been melted in previous quarters are measured using new mechanical testing machine, purchased in accordance to the project agreement (#3.7). Magneto-mechanical behaviour and effect of training on MFIS and martensitic structure has been studied as well (##3.7, 3.9). Theoretical study of magneto-mechanical behaviour of high temperature alloys based on the statistical theory of MFIS developed earlier will be continued in next quarters.

Microtwined martensite model of the Heusler alloys is developed (#3.8). This model for the first time gives the possibility for correct crystallographic description for all types of martensitic structures observed in the Ni-Mn-Ga alloys. Moreover, the model prognoses martensite and intermartensite transformations caused by change of the tetragonality ratio. Observed types of martensite structures can be explained and described as a variation of microtwinning of the basic tetragonal martensite structure. Correct crystallographic symmetry groups for martensitic structures are determined within the proposed model. The unit cell and atomic coordinates are calculated and constructed for tetragonal, 5M and 7M structures within the microtwins' model frame. The lattice parameters and their temperature dependence are calculated. Proposed model of microtwined martensite theoretically proves the growth of the martensite tetragonality with the rise of transformation temperature. This model is important for theoretical calculation of electronic and band structures, mathematical modelling of twin boundary motion, MFIS and martensitic transformation since it gives the correct crystallographic unit cells, atomic coordinates and corresponding lattice parameters. Twinning in 7M and non- modulated structures is studied (#3.8). We are preparing the article for publication concerned the new martensite microtwinning model.

According to the task (#3.5) the electronic structure was studied. It is experimentally shown that with the austenite-martensite phase transition, the magnetic moment of nickel atoms increases by $0.04\mu_B$ and those of the manganese atoms decreases by $0.03\mu_B$. As a consequence, the magnetic moment of whole unit cell increases by $0.05\mu_B$. Valence band of Ni_2MnGa intermetallics consists of two sub-bands. The first, pre-Fermi, is situated until ~ 10 eV below Fermi level for FCC and ~ 7 eV for BCT modification. The second, narrow band of deep states has binding energy near -14…-16 eV and is formed by gallium 3d-electrons. Pre-Fermi band is mainly formed by hybridised states of nickel and manganese atoms. Ni 3d electrons are dominant on the Fermi level. Large splitting of Ni and Mn electron states asserts their significant interactions. Interactions of gallium atoms with other alloy components are weakened. In Ni_2MnGa alloy dispersion laws are quite different for electrons with different spin directions. Band structures of FCC and BCT structures are very similar. Due to the theoretical study of electronic structure using experimental lattice parameters of Ni-Mn-Ga alloys in stoichiometric approximation it is shown that alloys possessing magnetic shape memory (MSM) and alloys without MSM have difference in the electronic structure. They differ in the occupation of 4s and 4p levels and in the splitting of 3d states of Ni and Mn atoms. Basing on the results of this study we proposed some mathematical function for description this difference. This function can be used as the awesome criteria to search for a new magnetic shape memory composition using the modelling methods (in case of its confirmation in our following studies for other experimentally studied compositions). We are preparing the article concerned the results have been obtained.

All results obtained for the Project during its first year of performance were analyzed. As the result we are preparing 4 articles mentioned above.

2. Summary of personnel commitment.

In sub-stages #2.1, 2.2 and #3.1 were involved: N. Glavatska, V. Gavriljuk (choice of chemical composition of polycrystals and melting and treatment routines), A. Urubkov, V. Bliznjuk (melting and specimen preparation), E.Tarusin (heat treatments). Single crystals were grown by I. Zasimchuk and L. Matvienko (#3.3). Tasks #3.1 and #2.2 are performed by I. Glavatskyy (determination of phase transformation temperatures by DSC and dilatometry) and A. Dobrinskiy (low-field magnetic susceptibility method). Effect of alloying by Fe on phase transformation temperature in Ni-Mn-Ga was studied by A. Dobrinskiy. Magnetic properties were studied by I. Glavatskyy and V. Bliznjuk (#2.3, 3.4). Mechanical testing of specimens was performed by I. Glavatskyy. V. Cherepin worked for optimisation of parameters of temperature controller for magnetic dilatometer. Magnetic field induced strain was measured by I. Glavatskyy and O. Rudenko (## 2.5, 3.6, 3.9). V. Lvov and O. Rudenko (modelling) studied a magneto-mechanical behaviour using the theoretical approach (# 3.9). Crystal structure of martensite in the single crystals was studied by N. Glavatska (X-ray diffraction), I. Glavatskyy (neutron diffraction) and V.Bliznjuk (transmission electron microscopy) (#3.6, #2.4). I. Surzhenko performed the orientation analysis of poly- and single- crystalline specimens by X-ray texture analysis, as well as studies of structure of polycrystals together with G. Mogilnyy (#3.6, #2.4). Studies of electronic structure (#2.6 та #3.5) were performed by I. Urubkov (experimental studies of austenite and martensite phase), V. Uvarov (computation of experimental spectra) and A. Urubkov (mathematic modelling). E. Bersudskiy was installing a special holder and temperature controller for the X-ray diffractometer. M. Knysh performed the technical maintenance of equipment and made some required metalworks and locksmithing. N. Glavatska has performed the scientific guidance, management, interpretation of the results and coordination of all project stages. We also invited some persons, who are not the project participants: chemical analysis was performed by V. Burtsev, I. Melnik melted the big-size polycrystals, V. Drobovich designed and manufactured a special holder for specimens for high-temperature studies with X-ray diffractometer.

3. Description of travels.

Mr. I. Glavatskyy held a travel to the Berlin Neutron Scattering Centre, Hahn-Meitner Institute (Berlin, Germany) in accordance with the project plan for the experiment with neutron diffraction study of the structure in new Ni-Mn-Ga alloys

4. Current status.

Scheduled tasks were performed according to project work-plan (tasks #2 and #3). Effect of alloying by Fe of the Ni-Mn-Ca compounds on the phase transformation temperatures is studied systematically. New perspective compositions of Ni-Mn-Ga and Ni-Mn-Ga-Fe alloys with high temperatures of martensitic transformation are found. Poly- and single crystals were melted and grown. Reorientation of twins' martensitic variants caused by the magnetic field is observed at 55^0C with value that corresponds to the magnetic field induced strain equal to 11%. Mechanical testing of new perspective alloys is done. A new theoretical crystallographicaly correct microtwins' model of martensite in Ni-Mn-Ga is developed. This model can be used for correct description of all martensitic structure types (either modulated or non-modulated), austenite–martensite and intermartensitic transformations. Crystallography of twinning for 7M martensite is studied. Electron and band structures of martensites with different lattice distortion were investigated. We proposed the mathematical function describing the electronic structure difference for different martensites. The function possibly could be used as a criterion in search for the new MSM alloys.
Automated device for the high temperature X-ray studies has been installed.
All results obtained for the Project during first year of the project performance were analyzed. As the result we are preparing for publication 4 articles mentioned above.

5. Problems encountered

Mechanical testing machine Hounsfield H1KT was purchased and installed according to the project work-plan (Annex 1 Table 4 #1). Paid for the construction of the specimen holder for high temperature X-ray studies. We paid to I. Melnik for melting the polycrystalline Ni-Mn-Ga-Fe ingot (140g weight), that is necessary for further single crystals growth with optimal composition. V. Burtsev (not a project participant) provided the chemical analysis of produced alloys. Printing accessories were purchased. Started the reconstruction in the new laboratory granted for the workgroup by the institute' administration. VSM magnetometer would be installed and adjusted after room reconstruction is complete. Thus, works planned for E. Bersudski in 4th quarter on magnetometer adjustment and repair will be transferred to the next quarter. For the reasons mentioned above the work time and money of the project participants were redistributed according to the letter L12, to provide the other important and complicated tasks. Details of the cost redistribution in the 4th quarter are presented in table below.

Table. Redirection

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)
L01 27.08.03	1. Diamond Cutting disks Tabl.4, #.17	411	1. Diamond Cutting disks Tabl. #.17	160	+251
	4. Memory DIMM 32 Mb SDRAM. Annex 1, Tabl. 4, #	0	4 .Memory DIMM 32 Mb SDRAM Winchester, Tabl.4 #11	120	-120
L04 23.09.03	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	1000		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	0	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	700	-700
	3. Travel to Sanct-Petersburg,	0	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	120	-120

	Russia, Tabl.8 #2				
	4. Travel to Kharkiv, Physical -Technical Institute, Tabl.8 #3	80	4. Travel to Kharkiv, Physical -Technical Institute, Tabl.8 #3	180	-180
	Total by 1Qv				$1411
	Redirection 2Qv				
L02 27.08.03	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder according to the project) Tabl.3, #.1.	150			+150
	2. Repairing/maintenance of equipment Tabl.7, # 6	0	2. Repairing/maintenance of equipment Tabl.7, # 6	150	-150
L03 27.08.03	1. N.Glavatska (Payment by cash for power supply temperature controller, Tabl.3, #.1	100			+100
	2. Power supply, Tabl. 7, # 20	0	2. Power supply for temperature controller Tabl. 7, # 20	100	-100
	2. Repairing/maintenance of equipment #6 Table 7	84	Repairing/maintenance of equipment #6 Table 7	150	-66
	Total 2 Qv				$316
Redirection 3 Qv					
L06 23.09.03	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1506	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1200	+306
	2. Travel to Berlin, Germany 2Qv #2,Tabl.8	0	2. Travel to Berlin, Germany, #2Tabl.	220	-220
	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	64	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	150	-86
	Total L06				306
L07 19.02.04	1. Adapter and Step down ring for optical microscope #21, Tabl.4	582	1. Adapter and Step down ring for optical microscope #21, Tabl.4	0	+582
	2. Voltage stabilisator #14, Tabl. 4	0	2. Voltage stabilisator #14, Tabl. 4	355	-355
	3. Communication (1-3Qv) #5,Tabl.7	0	3. Communication (1-3Qv) #5,Tabl.7	55	-55
	4. Chemical analysis (1Qv),#5,Tabl.7	0	4. Chemical analysis composition,(1Qv),#5,Tabl.	30	-30
	5.Computers (1Qv) ,##2-7,Tabl.4	3354	5.Computers (1Qv) ,##2-7,Tabl.4	3212	-142
	Total by L07				582
L08 23.02.04	1. N.Glavatska Tabl.3, #1	120	1. N.Glavatska Tabl.3, #1		+120
	2. Chemical analysis, Tabl. 7, # 11	0	2. Chemical analysis, Tabl.7, # 11	30	-30
23.02.02	3. Repairing/maintenance of equipment, Tabl.7,#8	60	3. Repairing/maintenance of an equipment, Tabl.7,#8	150	
	Total by L08				
L09 1.03.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L09 16.03.04	2. Special holder and device for diffractometer Tabl. 7, # 2	0	2. Special holder and device for diffractometer, Tabl. 7, # 2		-100
	Total by L09				100

Total 3Qv $1108

Redirection 4 Qv

L11 16.06.04	1. N.Glavatska Tabl.3, #1	110	1. N.Glavatska Tabl.3, #1		+110
	2. Chemical analysis, Tabl. 7, # 9	0	2. Chemical analysis, Tabl. 7, p 11	30	-30
	3. Repairing/maintenance of equipment, Tabl.7,#6	70	3. Repairing/maintenance of a equipment, Tabl.7,#8	150	-80
	Total by L11				110
L12 17.06.04	1. G. Mogylnyy Tabl.3, #15	500	1. G. Mogylnyy Tabl.3, #15	600	-100
	2. V.Bliznyuk Tabl.3, #16	270	2. V.Bliznyuk Tabl.3, #16	216	+44
	3. A.Rudenko Tabl.3, #17	240	3. A.Rudenko Tabl.3, #17.	210	+30
	4. I.Urubkov Tabl.3, #18	180	4.I.Urubkov Tabl.3, #17	216	-36
	5. I.Surzhenko Tabl.3, #19	342	5. I.Surzhenko Tabl.3, #19	144	+198
	6. A.Urubkov Tabl.3, #20	375	6. A.Urubkov Tabl.3, #20	255	+120
	7. E.Bersudskyy Tabl.3, #23	90	7. E.Bersudskyy Tabl.3, #23	306	-216
	8. I.Glavatskyy Tabl.3, #13	560	8. I.Glavatskyy Tabl.3, #13	600	-40
	Total by L12				648
	Total 4 Qv				$758

6. Delays and suggestions.

Due to the necessity of VSM magnetometer repair, that would be held after its' installation in the new lab, some delay in the magnetisation measurements of the new alloys is possible.

I ask your permission to use the money saved during the 1st year of the project performance in the next year for the purchase of needed equipment, especially for the defect-free single crystal cutting machine, defect-free chemical-mechanic polishing of the single crystals and also for purchase of the necessary components for magnetometer repair and portative copy-machine etc.

N.Glavatska

Project Manager

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

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Financing parties: USA, European Office of Aerospace Research & Development (EOARD)
Operative commencement date: 1 July 2004 - 30 September 2004
Project duration: 2 years
Date of submission: 20 October 2004

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1. Summary of progress.

Stage number and title	***#3 Optimization of compositions. Study of the constitution of the alloys having high temperatures of transformations***
Actual progress	Studies was directed on clarification of structure in the high temperature compositions in accordance with the project plan, investigation of the most important differences in the mechanical properties and crystal structure of alloys as well as factors affecting single crystals to display the magnetic shape memory. Comparative study of mechanical properties of alloys displaying the magnetic shape memory and without it is done (#3.7). Value of critical stresses needed for start motion of the twin boundary are determined as result of mechanical testing under compressive and tensile tests. It is shown that this value is about σ_{cr}=0,48 MPa for the best magnetic shape memory single crystals having 5-layered modulated structures. The strain maximum caused by the twin boundaries motion is equal 6,25% under compressive stress, 8,5Mpa at fixed temperature. Value of the non-reversible plastic strain is 4,5%. It is found that martensite in single crystals of some compositions of Ni-Mn-Ga display a **phenomenon of completely reversible linear super elastic strain- > 8% under stress 90MPa** (the picture illustrated result obtained is attached as a separately file). <u>Possibility to patent alloys with an effect of linear giant super elasticity is investigated.</u> A physical mechanism of that kind of super elasticity is not clear this time. Study of the magnetic field induced strain has shown that alloys having modulated 5- or 7 layered structured (5M or 7M) display the magnetic shape memory and giant magneto-plasticity. Alloys having the non-modulated tetragonal structure do not show magnetic field induced strain under magnetic field equal to a magnitude of the magnetic field saturation. Compositions having 5M modulated structures have the highest tendency to the magneto-plasticity. But unfortunately they have not enough high temperatures of martensite transformation ($\leq 45^0$C). Effect of magnetic field induced strain in the studied 7M modulated mertensites (Table 3 and report for 4 Qv) is unstable and value of measured MFIS is smaller than theoretical maximum at fixed temperature. Composition having mixed 5M and 7M structures (Tabl. 3).are selected fs some perspective compositions of the high temperature Ni-Mn-Ga alloys. Also we have found that conditions of single crystal grown, previous treatments, procedures of specimen performance and cooling rate during the direct martensite transformation affect the critical magnetic field value and value of MFIS. This study will be continued systematically during 6 Qv.

Details of the crystal and magnetic structure, pecular to the best single crystals showing highest magnetoelasicity at the lowest magnetic field, were studied by using neutron diffraction and transmission electron microscopy in the single crystal y $Ni_{48,57}Mn_{30,14}Ga_{21,4}$ (#3.8). Studied single crystal has MFIS value 4,3% at 33^0C (0,18T) at 0,18T that is almost close to the theoretical limit at this temperature/ Chemical composition in the bulk crystal was determined by using a fluarescent method of analysys. As follows from the neutron diffraction study, the bulk single crystal specimen has 5M structure. Evolution of crystal and magnetic structure with temperature was studied using 4-circle neutron diffractometer (ILL, Grenoble, France). Details of magnetic and crystal structure were studied under cooling down because study of magnetic structure is possible at low temperature only using cryomagnet. It was found that crystal structure is orthorhombic above 175^0C with the *Immm* space grope. Crystal structure becams to be monoclinic with cooling down below 175^0C (Tabl.1).

Table 1. Lattice parameters of $Ni_{48.5}Mn_{30.14}Ga_{21.4}$.

T, K	a, Å	b, Å	c, Å	α, °	β, °	γ, °	Deviation, °
298	4.2102 (0.0005)	5.6181(0.0009)	20.993(0.003)	90	90.07 (0.01)	90	0.0568
175	4.215 (0.003)	5.534(0.003)	20.956(0.009)	90	90.09 (0.03)	90	0.0466
20	4.209 (0.002)	5.519(0.004)	20.951(0.008)	90	90.20 (0.03)	90	0.0522

Non-monotonous dependence of the peak intensity on temperature is found for some selected diffraction peaks. Temperature evolution of 11 peaks was studied within the temperature range 300-10K with step of measurement of temperature 25K. of Stability of (1 -3 0) and (0 0 10) peaks with cooling was observed. It is non-ordinary fact because of difference in the nature of these peaks: (0 0 10) peak has strong magnetic component to compare with (1 -3 0) peak, which has small magnetic component (only 2/3 μB take part in the magnetic scattering). Some anomalies in the scattering are found: rise of integral intensity of magnetic peaks within temperature range 300-220K. All together 107 peaks having high intensity and 609 peaks with low intensity were studied. The completely data handling for the magnetic structure determination needs to make some change in the program software and large calculation time therefore it will be continued in the next future.

Study of the crystal structure using the transmission microscopy method in the thin foil prepared from the bulk single crystal mentioned above, shows that there are some notably differences in the martensitic structure in the bulk specimen and foil. The 4 various crystal structure types are observed in the foil: 1) twinned martensite having modulated 5M structure; 2) twinned martensite having modulated 7M structure; 3) martensite combined from intersected stacking faults; 4) non- modulated tetragonal martensite. The lattice parameters for all these structure types are determined. The local chemical analysis in the areas corresponding to these four crystal structure types was performed using the EDX spectroscopy method (Tabl.2). As follows from the Tabl. 2, areas having different crystal structure types have almost the same composition. That shows co-exististence of various types of crystal structures having the same Ni, Mn and Ga content in foils. It was known until now from a literature that type of crystal structure depends on chemical composition. Difference in composition and transformation temperatures in bulk specimens having tetragonal and modulated structures is quite big (percents, see as example Tabl.3). **We have shown that not only composition affects on type of martensite structure in Ni-Mn-Ga but the size factor also**. That result can explain some differences taking place in the literature published by various authors concerning interrelation between composition and structure in Ni-Mn-Ga. It means necessity take into account an effect of the size factor to analyze effect of composition on the structure type. We start to prepare an article concerned on these results obtained.

Table 2. Structure and chemical composition in the foil of the crystal

Zone	Structure of martensite	Ni, ат.% ±ат.%	Mn, ат.% ±ат.%	Ga, ат.% ±ат.%
1	5M twinned	47,67 ±0,04	31,16 ±0,1	21,17 ±0,07
2	7M twinned	48,01	30,76	21,23
3	Non-modulated tetragonal	47,8 ±0,11	30,87 ±0,09	21,34 ±0,03

It is found that 5M and 7M martensites are twined on the micro- structure level. Non- modulated tetragonal martensite with the same composition in foil as well as tetragonal martenstite in high temperature bulk single crystal has no micro-twins. Its structure consists intersected staking faults and structure of tweed type as well. That structure has *CzCl* like type of ordering what is different to compare with 5M and 7M structures

Study of possibility to obtain MFIS in the stress-induced martensite was continued for thew allos having tempreatures martensite transformation >70^0C and non-modulated teragonal m thermal martensite in the bulk specimens. The alloy with composition Ni53,3 Mn19,1Ga 23.6 having temperature of martensite transformation M_f=77^0C was studied. Another type of the stress-induced martensite was obtained due to the thermo-mechanical cycling. That martensite has monoclinic type of a structure. This type of martensite does not show magneto-plasticity under magnetic field up to field of saturation to compare with the stress-induced martensite in the alloy with higher Mn content (Ni53,9 Mn24,4Ga 21.7) studied in the 4 quarter.

An effect of rate of the magnetic field and stress application on the stability of magnetic field or stress induced strain is found. Dependence of magnitude and critical value of magnetic field or stress (#3.7 on stress/field application is studied as well. We are going to continue study of that effect systematically with a goal to take stable magnetic actuating elements.

Poly- and single crystals of Ni-Mn-Ga-X ingots with improved compositions were melted and grown (##3.1-3.3). New compositions alloyed by Si and Sn have the higher temperatures of martensite transformations to compare with alloys studied in the previous quarter and that reported in the literature. Effect of technological parameter of the crystal grown was studied with a goal to improve quality of single crystals. It is shown, that increase of time for the single crystal crystallization causes improving of quality. However, more long time of duration of stay at high temperature causes loosing of Mn. It affects the final composition of single crystal and, correspondently, temperatures of martensite transformation (to compare Ju68 та 68b_z1, Табл.3). It means necessity to increase Mn content in the compositions for melting of polycystals and followed single crystal grown. (Loosing of Mn during thermal treatments is studied in previous quarters). Temperatures of the phase transformation and structure in new alloys are studied (Table 3).

Table 3. Хімічний склад, температури фазових перетворень та структури монокристалів

	at%				^0C					Structure
Name	*Ni*	*Mn*	*Ga*	*X*	*Tc*	M_S	M_f,	A_s	A_f	
Ju68 *Single crystal (slow)*	*46.5*	*23.7*	*29.7*	-	***106***	***68***	***59***	***77***	***85***	*7M, Tetragonal non-layered*
68b_z1 *Single crystal (4Qv fast")*	***45,50***	***33,87***	***20,62***	-	***85,9***	***57,5***	***50,5***	***51,6***	***59,2***	*7M, 5M*
N5_AF *Single crystal*	**48,07**	**29,28**	**20,45**	**Al** 1,16 **Fe** 0,33	***122,4***	***61***	***45,6***	***45,6***	***61***	*5M+7M*
N5-Fe *Single crystal*	*47,34*	*25,86*	*20,38*	Fe 6,42	*99,6*	*22,8*	*3,4*	*4,5*	*29,8*	‘
j0704a *Polycrystal*	50,7	30,2	18,1	Si 1,0 Fe 0,37	*103.4*	*22.2*	*12.8*	*20.1*	*30*	‘
j0704c *Polycrystal*	**50**	**29,8**	**17,1**	**Si 3,1**	***100***	***27.2***	***20.6***	***26.4***	***35***	‘
j0104c	***50***	***28,0***	***20,8***	***Sn 1,0***	***90.5***	***28.4***	***22.5***	***24***	***30.9***	‘

*will be studied

It is shown that rate of cooling during the single crystal grown also affects type of crystal structure (Table 3), as well as alloys composition and the size factor discussed above.

Decreasing of the critical magnetic field needed for magneto-plasticity due to the twin boundary motion with the temperature rise (founded experimentally early) is studied theoretically (#3.9). This study is important to understand processes affected magneto-plasticity at higher temperatures. Two different factors affect an effect mentioned above are investigated: the temperature dependence of magnetization and temperature dependence of the pinning effect on the twin boundary motion. Comparison of theoretical and experimental results is done for Ni-Mn-Ga-Fe (ApFe2, Tabl. 1, reported in Q04). Rise in the critical magnetic field from 0,55T down to 0,52T at rise temperature from 23^0C up to 45^0C is analysed. Rise of temperature affects decrease in the equivalent stresses caused by the magnetic field. The most effective field decrease is observed at temperatures close to the Curie temperature. That fact shows importance to find compositions having not only higher the martensite transformation temperatures but higher Curie temperature as well.

An important result is obtained due to the comparative analysis of an electronic structure in the magnetic shape memory alloys and alloys, which do not show magneto-plasticity (#3.5). We have found that there are some crystallographic planes and directions in the magnetic shape memory alloys having lower level of the free electron density localization, what can be a reason of higher instability of structure in these directions, including instability under magnetic field and/or mechanical stress.

2. Summary of personnel commitment.

In sub-stage #3.1 were involved: N. Glavatska, V. Gavriljuk (choice of chemical composition of polycrystals and melting and treatment routines), A. Urubkov, V. Bliznjuk, A.Dobrinskiy (melting and specimen preparation), E.Tarusin (heat treatments). I. Zasimchuk and L. Matvienko have grown single crystals (#3.3). Tasks #3.1 and 3,2 were performed by I. Glavatskyy (determination of phase transformation temperatures by

DSC and dilatometry) and A. Dobrinskiy (low-field magnetic susceptibility method. I.Glavatskyy and A.Rudenko performed mechanical tests (# 3. 7). I.Glavatskyy and I.Urubkov are studied of magnetic structure by means of neutron diffraction method (# 3. 4). Magnetic field induced strain is studied by A.Rudenko and .lGlavatskyy (# 3.7). V.Lvov has made a theoretical analysis of temperature dependence of magnetization and MFIS (# 3.9). Crystal structure is studied by N.Glavatska (x-ray diffraction of single crystals), I,Glavatskyy (neutron diffraction of single crystals), V.Bliznjuk (transmission electron microscopy), G,Mogilnyy (x-ray diffraction of poly- and single crystals) (#3.6). I.Surzhenko performed orientation of single crystals by using x-ray diffraction texture analysis (#3.6). V.Uvarov and A.Urubkov studied an electronic structure (#3.5). E.Bersudskiy made testing of magnetometer. M. Knysh performed the technical maintenance of equipment and made some required metal works. V.Isyanov constructed an special device for magnetization and re-magnetization of specimens. N.Glavatska analysed all results obtained and managed the project performance.

3. Description of travels.

Mr. I. Glavatskyy and Mr. I.Urubkov had a travels to the Institute Laue-Langevin (ILL) Grenoble, France) to stud y of crystal and magnetic structure by means 4-circle neutron diffractometer. N.Glavatska held travel to Mexico to participate in the Symposium “ Magnetic shape memory alloys” with an invited lecture.

4. Current status.

Scheduled tasks are performed according to the project work-plan (tasks #3). Comparative study of mechanical properties of the magnetic shape memory crystals with 5M and 7M crystal lattice and alloys without magneto-plasticity with tetragonal structure is done. Phenomenon of completely reversible linear super plasticity equal 8% at mechanical stressing of 90MPa is found. New perspective compositions of poly-crystals Ni-Mn-Ga, alloyed by Al, Fe, Si, Sn having higher transformation temperatures are melted. Effect of crystallization rate on single crystal quality, chemical composition and crystal structure is studied. It is shown that type of crystal structure depends not only on chemical composition, as it suggested in a literature, but on size factor and on rate of crystallization and followed treatments. Magnetic structure in the magnetic shape memory single crystals is studied. Some temperature anomalies in the magnetic structure are found. Explanation of this fact needs additional studies. Study of magneto-plasticity in the stress-induced martensite of high temperature alloys was continued. Decrease of critical magnetic field at elevating temperature is studied theoretically. The most effective decrease in the critical field is at temperature close to the Curie temperature. Due to study of an electronic structure, we have found that there are some special crystallographic planes and direction in the magnetic shape memory alloys having lowest value of free electrons localization, A patent concerned on the phenomenon of linear super-elasticity in the martensitic phase is prepared.

5. Problems encountered. We have bought a new computer and permanent magnets Nd-Fe-B for studies. Repairing of the room for researchers involved to the project is finished. Due to travel to Laue-Langevin (ILL) Grenoble, Francecrystal and magnetic structure in the magnetic shape memory single crystal is studied. Professor V.Gavriljuk does not participate in the project starting from August. A new participant Mr. V.Isyanov is involved to the project. Some redirection of the work time between project participants was made to optimize studies for the project during the summer holiday period. Table below explains details of redirections.

Table. Redirection.

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (ne w-old)
	Redirection 1 Qv				
L01 *27.08.03*	*1. Diamond Cuting disks* Tabl.4, #.17	*411*	*1. Diamond Cuting disks Tabl.4 #.17*	160	*+251*
	4. Memory DIMM 32 Mb SDRAM. Annex 1, Tabl. 4, #	*0*	*4 .Memory DIMM 32 Mb SDRAM Winchester, Tabl.4 #11*	*120*	*-120*
L04 *23.09.03*	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	*1000*		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	*0*	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	*700*	*-700*

	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	*0*	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2		*-120*
	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	*80*	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	*180*	*-180*
	Total by 1Qv				*1411*
	Redirection 2 Qv				
L02 *27.08.03*	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder according to the project) Tabl.3, #.1.	150			*+150*
	2. Repairing/maintenance of equipment Tabl.7, # 6	*0*	*2. Repairing/maintenance of equipment Tabl.7, # 6*	150	*-150*
L03 *27.08.03*	1. N.Glavatska (Payment by cash for power supply temperature controller, Tabl.3, #.1	*100*			*+100*
	2. Power supply , Tabl. 7, # 20	*0*	2. Power supply for temperature controller Tabl. 7, # 20	*100*	*-100*
	2. Repairing/maintenance of equipment #6 Table 7	*84*	Repairing/maintenance of equipment #6 Table 7	*150*	*-66*
	Total 2 Qv				*$316*
Redirection *3 Qv*					
L06 *23.09.03*	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	*1506*	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1200	*+306*
	2. Travel to Berlin, Germany 2Qv #2,Tabl.8	*0*	2. Travel to Berlin, Germany, #2Tabl.	*220*	*-220*
	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	*64*	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	*150*	*-86*
	Total L06				*306*
L07 *19.02.04*	1. Adapter and Step down ring for optical microskope #21, Tabl.4	*582*	1. Adapter and Step down ring for optical microskope #21, Tabl.4	0	*+582*
	2. Stabilisator of voltage #14, Tabl. 4	*0*	2. Stabilisator of voltage #14, Tabl. 4	*355*	*-355*
	3. Communication (1-3Qv) *#5,Tabl.7*	0	3. Communication (1-3Qv) *#5,Tabl.7*	55	-55
	4. Chemical analysis (1Qv),#5,Tabl.7	0	4. Chemical analysis composition,(1Qv),#5,Tabl.	30	-30
	5.Computers (1Qv) ,##2-7,Tabl.4	3354	5.Computers (1Qv) ,##2-7,Tabl.4	3212	-142
	Total by L07				582
L08 *23.02.04*	*1. N.Glavatska* Tabl.3, #1	*120*	*1. N.Glavatska* *Tabl.3, #1*		*+120*
	2. Chemical analysis, Tabl. 7, # 11	*0*	2. Chemical analysis, Tabl.7, # 1	*30*	*-30*
23.02.02	3. Repairing/maintenance of equipment, Tabl.7,#8	60	3. Repairing/maintenance of an equipment, Tabl.7,#8	150	
	Total by L08				
L09 *1.03.04*	*1. N.Glavatska* Tabl.3, #1	*100*	*1. N.Glavatska* *Tabl.3, #1*		*+100*

L09 16.03.04	2. Special holder and device for diffractometer Tabl. 7, # 2	*0*	2. Special holder and divice for diffractometer, Tabl. 7, # 2		-100
	Total by L09				100
	Total 3Qv				1108
Redirection 4 *Qv*					
L11 16.06.04	*1. N.Glavatska* Tabl.3, #1	*110*	*1. N.Glavatska Tabl.3, #1*		*+110*
	2. Chemical analysis, Tabl. 7, # 9	0	2. Chemical analysis, Tabl. 7, p 11	30	-30
	3. Repairing/maintenance of equipment, Tabl.7,#6	70	3. Repairing/maintenance of a equipment, Tabl.7,#8	150	-80
	Total by L11				110
L12 17.06.04	1. G. Mogylnyy Tabl.3, #15	*500*	*1. G. Mogylnyy Tabl.3, #15*	600	*-100*
	2. V.Bliznyuk Tabl.3, #16	*270*	*2. V.Bliznyuk Tabl.3, #16*	216	*+44*
	3. A.Rudenko Tabl.3, #17	240	3. A.Rudenko Tabl.3, #17.	210	*+30*
	4. I.Urubkov Tabl.3, #18	*180*	*4.I.Urubkov Tabl.3, #17*	216	*-36*
	5. I.Surzhenko Tabl.3, #19	342	5. I.Surzhenko Tabl.3, #19	144	+198
	6. A.Urubkov Tabl.3, #20	375	*6. A.Urubkov Tabl.3, #20*	255	+120
	7. E.Bersudskyy Tabl.3, #23	90	*7. E.Bersudskyy Tabl.3, #23*	306	-216
	8. I.Glavatskyy Tabl.3, #13	560	*8. I.Glavatskyy Tabl.3, #13*	600	-40
	Total by L12				648
	Total 4 Qv				758
	Redirection *5 Qv*				
L10 15.06.04	1. Travel to Institute Laue-Langevin ILL (Grenoble, France) for the neutron diffraction experiment	1150	1. Tabl.8,	0	+1150
	2. Travel to Berlin, Germany 4Qv #2,Tabl.8	190	2. Travel to Berlin, Germany, #2Tabl 8.	340	-150
	3. Travel for the EPDIC -9 conference, #1,Tabl.8	*0*	3. 3. Travel for the EPDIC -9 conference, #1,Tabl.8	1000	-1000
	Total by L10				**1150**
L13 17.06.04	*1.Computers (Non-Capital) Tabl.4,# 1-7*	*5012*	*1.Computers (Non-Capital)* Tabl.4,# 1-7	4354	+658
	2.. Portative Mechanical testing Machine, *Tabl.4,# 1*		2. Portative Mechanical testing Machine, Tabl.4,# 1	18000	-658
	Total by L13				658
L14 21.06.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L14 21.06.04	2. Repairing of a room Tabl.7,#11	0	2. Repairing of a room, Tabl.7,#11	100	-100
	Total by L14				100
L15 08.07.04	1. Travel to Cancun for Symposium on "Magnetic Shape Memory Alloys", Tabl.8,	937		0	+937
	2. Travel to France for ESOMAT conference, Tabl.8 #5	63	2. Travel to France for ESOMAT conference, Tabl.8 #5	1000	-937
	Total by L15				937
L16	1. V.Gavruljuk (Tabl.3#1)	2790	1. V.Gavruljuk (Tabl.3#1)	5010	-2220

15.07.04		1-5 Qv		1-8 Qv	
	2. V. Is’yanov (Tabl.3 #19)	2220 5-8 Qv	2. V. Is’yanov (Tabl.3, #19)	0 5-8 Qv	+2220
	3.E.Bersudskyy (Tabl 3#18)	0 4 Qv	3. 3.E.Bersudskyy (Tabl 3#18)	108 4 Qv	-108
	4.E.Bersudskyy (Tabl 3#18)	108 5 -6Qv	3. 3.E.Bersudskyy (Tabl 3#18)	0 5-6 Qv	+108
	Total by L16				2328
L17 01.09.04	1. I.Zasimchuk (Tabl.3#3)	400 5 Qv	1. I.Zasimchuk (Tabl.3#3)	500 5 Qv	-100
	2. Artem.Urubkov (Tabl.3 #15)	330 5 Qv	2. A.Urubkov (Tabl.3 #15)	240 5 Qv	+90
	3.I Surzenko (Tabl 3#14)	216 5 Qv	3. I Surzenko (Tabl 3#14)	144 5 Qv	+76
	4. Ilya Urubkov (Tabl.3 #15)	180 5 Qv	4. Ilya Urubkov (Tabl.3 #15)	216 5 Qv	-36
	5.V.Gavriljuk (Tabl.3#2)	300 5 Qv	5.V.Gavriljuk (Tabl.3#2)	630 5 Qv	-330
	6. V.Isyanov (Tabl.3#19, New participant)	300 5 Qv	6. V.Isyanov (Tabl.3#19)	0 5 Qv	+300
	7. V.Cherepin (Tab3.5#5)	0 5Qv	7. V.Cherepin (Tab3.5#5)	250 5Qv	-250
	8. V.Cherepin (Tab3.5#5)	250 6Qv	8. V.Cherepin (Tab3.5#5)	0 5Qv	+250
	9. V.Uvarov (Tabl.3#11)	9	10. V.Uvarov (Tabl.3#11)	350 5 Qv	-175
	10. V.Uvarov (Tabl.3#11)	175 7 Qv	10. V.Uvarov (Tabl.3#11)	0 7 Qv	+175
	Total by L17				891
	Total 5 Qv				5994

6. Delays and suggestions.

Studies are performed in accordance with the project plan.

N.Glavatska

Project Manager

P-137, Q05.

Super elastic absolutely reversible strain in the Ni-Mn-Ga.

Figure 1 illustrates the super elastic absolutely reversible strain in the new Ni-Mn-Ga crystal. Figure 2 showing an example of well known strain-stress curves in the Ni-Mn-Ga single crystals is given for comparison with the Fig.1.

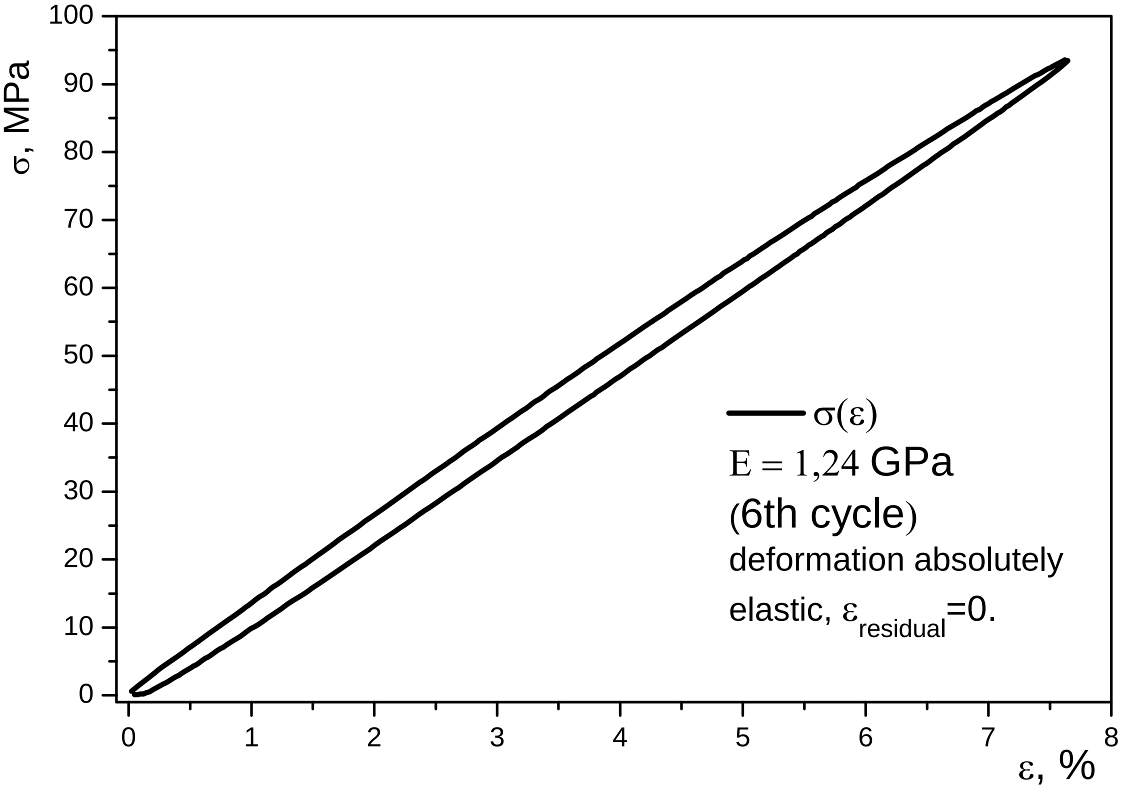

Fig 1. Super elastic reversible strain in the Ni_x-Mn_y-Ga_z single crystal.

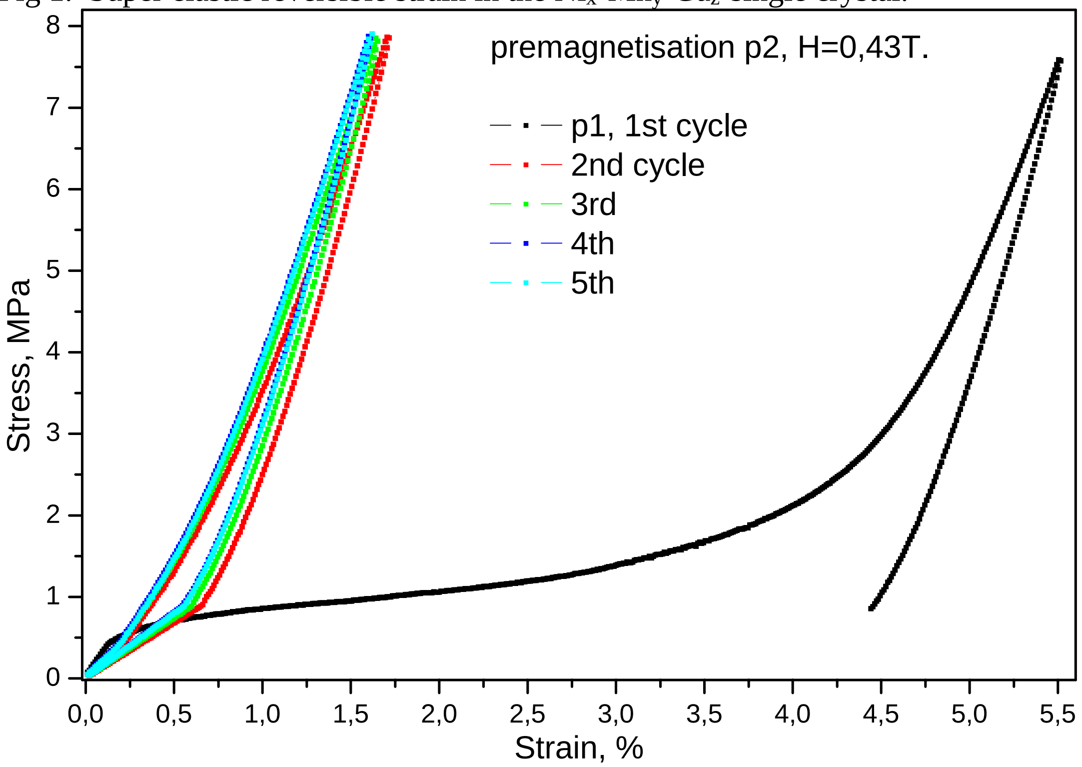

Fig.2. Strain under stress in the $Ni_{48,57}Mn_{30,14}Ga_{21,4}$ magnetic shape memory single crystals: black line- along the axis of easy magnetization, colour lines- along the “hard” axis.

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

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Financing parties: USA, European Office of Aerospace Research & Development (EOARD)
Operative commencement date: 1 July 2004 - 30 September 2004
Project duration: 2 years
Date of submission: 23 January 2005

1. Summary of progress.

Stage number and title	***#3 Optimization of compositions. Study of the constitution of the alloys having high temperatures of transformations***
Actual progress	Studies were performed in accordance with the project plan (#3) and directed on optimization of compositions of the Ni-Mn-Ga+X alloys having temperatureof the martensitic transformation well above room temperature and optimal type (5- or 7- layered modulated) of the crystal lattice in martensite. As we have found in previous quarters, only alloys having of the multilayered modulated type of the crystal structure (5M, 7M) can display the magnetic field induced strain in the martensitic phase. Martensite with non- modulated tetragonal structure do not show the magnetic field induced strain until the magnetic field values equal to the saturated magnetization due to low mobility of the twin boundaries. Martensites with 5M modulated structure have the highest mobility of the twins and turn for the magnetic shape memory. New poly – and single crystals of Ni-Mn-Ga-X with different composition were melted (##3.1-3.3). Compositions were optimized basing on the data of the study in the stage #2 on the one hand and absolutely new compositions were searched on the other hand. Correlation between an electronic structure (the valence electron density), an atomic (covalent) radius of the alloyed element and the magnetic and martensitic transformation temperatures in Ni-Mn-Ga-X compositions were studied (#3.5). Choice of the new alloying elements for new composition was done basing on our fundamental study performed in the project frame. Due to that study we selected a few new elements promising to increase the martensitic transformation temperatures in Ni-Mn-Ga. The main consideration was given to optimize compositions alloyed by Fe. One of the reasons of this particular attention to alloying by Fe is a lower price of the new high temperature magnetic shape memory actuators alloyed partially by Fe instead of the very expensive Ga. As result, we have found the new compositions of Ni-Mn-Ga alloyed by Fe

having optimal temperatures of the martensitic transformations (Table 1). The alloy № 3 was melted in the previous quarter. We have studied its crystal structure in the current quarter. The crystal structure of new alloys was studied as well (Table 1).

Table 1. Content and transformation temperatures of new compositions alloyed by Fe

N	Ni at%	Mn at%	Ga at%	Fe at%	T_c at%	M_S ^{0}C	M_f, ^{0}C	A_s ^{0}C	A_f ^{0}C	Structure
3	49,42	27,62	21,34	1,79	113	43	55	54	59	5M
8	51.33	14.44	26.27	7.95	115.8	85.7	78.8	88.2	101	5M+7M
6	52,15	16,96	21,26	9,63	115,5	108,2	96,6	99,9	115	7M+ NT (+ 2 phase)

It is found that in the case of alloying by Fe, alloys having the transformation temperatures ratio M_s/Tc>1 (Tc- Curie temperature, Ms- temperature of start of the direct martensitic transformation) have non- modulated crystal type of the martensitic structure and do not display magnetic shape memory. That confirms our conclusion we made in the previous quarter for the Ni-Mn-Ga alloys. Compositions alloyed by Fe with M_s/Tc <1 have 5- or 7- layered type of martensitic structure and turn for magnetic field induced strain (Table 1, №3,8). Moreover, we have found that alloying by Fe causes rise in the temperature of ferromagnetic transformation. That means alloying by Fe increases the temperature interval of the modulated structures existence and causes some shift of temperatures of application to the higher temperatures what is important for practical application that is the main goal of the project.
It is shown for Fe-alloyed Ni-Mn-Ga that if difference between Curie temperature and the martensitic transformation temperature in small, the 7-layered modulated structure of martensite is observed (Table 1) as well as in the poor Ni-Mn-Ga alloys. Alloy №6 with Fe content 9,63% have in the martensitic state co-existence of two phases. One of them has mixed structure: 7-layered modulated structure co-exists with the non-modulated tetragonal type of crystal structure. Optimization of treatments for that alloys with a goal to obtain one-phase state in this martensite (Table 1, №6) requires of some additional investigations.
We continue searching of a new perspective alloying elements for the new high-temperature compositions of Ni-Mn-Ga based alloys, corrections of they're content and study effect of alloying on transformation temperatures (##3.1-3.3). Basing on that study we have found firstly the new perspective compositions of Ni-Mn-Ga alloyed by Cu. It was melted 5 compositions Ni-Mn-Ga-Cu. Table 2 shows the best alloys with Cu we have found. These alloys have high temperatures of martensitic transformation, good Tc/Ms ratio. Therefore alloying by Cu seems to be perspective for following studies. As have shown study of magnetic properties all these alloys are ferromagnetic and have strong magnetic anisotropy (#3,4).

Таблиця 2.

N	Ni at%	Mn at%	Ga at%	X	X. at%	Tc.°C	M_s °C	M_f °C	A_s °C	A_f °C	Structure
17a	49.36	27.798	20.863	Cu	1.98	88.9	85.9	70.5	89.4	106.6	7M
17b	49.64	27.558	18.922	Cu	3.89	117.5	115	97.8	121.6	150	7M+ NT
23In2	48.94	24.75	22.90	In	3.41	84.2	5.6	-17.5	-3.1	16	*

Study of the crystal structure by means of x-ray diffraction (#3,6) has shown that in the case of alloying by Cu the correlation of Tc/Ms ratio and the crystal structure type is observed as well as in the case of Ni-Mn-Ga and Ni-Mn-Ga-Fe. It indicates a general character of that correlation. The 7-layered modulated structure exists in the 17a та 17б alloys (Табл.2). Therefore at least one of these alloys (17a) will be studied in the single crystal state as some main candidate for high temperature magnetic shape memory alloys. Let as note that substitution of Ga on Cu also causes reducing in price of alloys notably. Measure of the magnetic field induced strain in this selected Cu-alloyed Ni-Mn-Ga (17a) will be done in the 7 quarter.

Also we studied effect of alloying by In on the martensitic transformation temperatures in Ni-Mn-Ga. Table 2 represents the best composition with In, which we have found. Alloying by In seems not so interesting for the project goal to compare with Fe and Cu alloyed Ni-Mn-Ga.

We continued optimization of the single crystal grown conditions to improve they're quality. (#3,2). Search of better conditions for the single crystal grown is done for the selected high-temperature Ni-Mn-Ga and Ni-Mn-Ga-Fe single crystals and melted in the previous quarter.

Study of an effect of the application rate of the magnetic field and compressive stress on the magnetic field/stres induced strain was continued. Study of that effect at higher temperatures is started for Ni-Mn-Ga (#3.7). Rate of the applied magnetic field or a compressive stress effects value of the magnetic field /stress induced strain, however this effect having not a single meaning. It depends on previous history of a specimen and degree of sophistication of the single crystals.

Basing on our previous study (Glavatska N. I., Rudenko A. A., Glavatskiy I. N., L'vov V. A., Statistical model of magnetostrain effect in martensite. *JMMM*, **265**, 142 (2003) an effect of thermal fluctuationon the magnetic field induced strain and thay're role in the temperature dependence of the magnetic field induced strain and magnetization in Ni-Mn-Ga-Fe martensites is studied theoretically (# 3.9). Article concerned results of that study is ready to submit its for publication.

Device for cycled magnetization of the specimens is made. Its construction is optimized and improved.

2. Summary of personnel commitment.

N. Glavatska, I. Urubkov, V. Bliznjuk, A.Dobrinskiy I.Glavatskiy were involved in study in accordance with sub-stage #3.1 (choice of chemical composition of polycrystals, melting of alloys, specimen preparation) and E.Tarusin (heat treatments). I. Zasimchuk and L. Matvienko have grown single crystals and optimized the grown routines (#3.3). Tasks #3.1 and 3,2 were performed by I. Glavatskyy and A. Dobrinskiy (determination of phase transformation temperatures by DSC, dilatometry and with low-field magnetic susceptibility methods.). I.Glavatskyy and I. Urubkov are studied of magnetic properties and magnetic structure by means of the magnetization study and neutron diffraction method and (# 3. 4). V. Lvov has performed theoretical analysis of temperature dependence magnetization and magnetic field induced strain in Ni-Mn-Ga alloyed by Fe (# 3.9). N/Glavatska studied the crystal structure of martensite in the Cu- containing martensites by means X-ray diffraction single crystal analysis (#3.6). I.Surshenko and G.Mogylnyy studied the phase content in the new polycrystalline alloys with X-ray diffraction method. They both also performed orientation of single crystal by using texture analysis. V.Uvarov and I.Urubkov studied preliminary effect of alloying by Fe and Cu on the electronic structure of Ni-Mn-Ga (Fe, Cu) austenite (#3.5). M. Knysh performed the technical maintenance of equipment and made some required metal works. V.Cherepin and V.Isyanov take main part in the construction and making of an special device for cycled magnetization and re-magnetization of specimens. N.Glavatska analysed all results obtained and managed the project performance.

3. Description of travels.

We have no travels in 6 quarter.

4. Current status.

Scheduled tasks are performed according with the project plan (tasks #3). The main result of study in the current quarter are following: basing on the fundamental studies (electronic structure, crystal structure and they're correlation with the transformation temperatures and magnetic field induced strain) a new alloyed elements are found; content of alloyed compositions is optimized; a new Ni-Mn-Ga-Cu alloy shoving high temperatures of martensitic transformation (75^0C), modulated crystal structure type and strong magnetic anisotropy is found, what is necessary condition to display magnetic shape memory at higher temperatures.

5. Problems encountered.

It is paid ($1809) for construction and crating of machine for chemical cutting of single crystals in accordance with letter (L18). We have bought the Scanner HP-Scan-Jet ($79,6) using money saved in the previous quarters, the Hard Disk HDD 40 Gb for the computer instead of the brooked ones ($111,5) and flexi force devices for the mechanical testing machine ($168).

The project participant O.Rudenko has gone to Israel for long time business travel therefore he does not take part in the project performance. Work planed for O.Rudenko and his grant for the 6 quarter were redirected to A.Urubkov, I.Surshenko and A.Dobrinskiy.

Then the project participant A.Urubkov has gone to Russia for the permanent leaving and does not take part in the project. Work planed for A.Urubkov and his grant for the 6 quarter were redirected to I.Urubkov, A.Dobrinskiy, I.Glavatskiy and N.Glavatska. Table below explains all details of redirections.

Table. Redirection.

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (ne w-old)
	Redirection 1 Qv				
L01 27.08.03	1. Diamond Cuting disks Tabl.4, #.17	411	1. Diamond Cuting disks Tabl.4 #.17	160	+251
	4. Memory DIMM 32 Mb SDRAM. Annex 1, Tabl. 4, #	0	4 .Memory DIMM 32 Mb SDRAM Winchester, Tabl.4 #11	120	-120
L04 23.09.03	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	1000		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	0	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	700	-700
	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	0	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2		-120
	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	80	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	180	-180
	Total by 1Qv				1411
	Redirection 2 Qv				
L02 27.08.03	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder according to the project) Tabl.3, #.1.	150			+150
	2. Repairing/maintenance of equipment Tabl.7, # 6	0	2. Repairing/maintenance of equipment Tabl.7, # 6	150	-150
L03 27.08.03	1. N.Glavatska (Payment by cash for power supply temperature controller,	100			+100

	Tabl.3, #.1				
	2. Power supply , Tabl. 7, # 20	0	2. Power supply for temperature controller Tabl. 7, # 20	100	-100
	2. Repairing/maintenance of equipment #6 Table 7	84	Repairing/maintenance of equipment #6 Table 7	150	-66
	Total 2 Qv				$316
Redirection 3 Qv					
L06 23.09.03	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1506	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1200	+306
	2. Travel to Berlin, Germany 2Qv #2,Tabl.8	0	2. Travel to Berlin, Germany, #2Tabl.	220	-220
	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	64	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	150	-86
	Total L06				306
L07 19.02.04	1. Adapter and Step down ring for optical microskope #21, Tabl.4	582	1. Adapter and Step down ring for optical microskope #21, Tabl.4	0	+582
	2. Stabilisator of voltage #14, Tabl. 4	0	2. Stabilisator of voltage #14, Tabl. 4	355	-355
	3. Communication (1-3Qv) #5,Tabl.7	0	3. Communication (1-3Qv) #5,Tabl.7	55	-55
	4. Chemical analysis (1Qv),#5,Tabl.7	0	4. Chemical analysis composition,(1Qv),#5,Tabl.	30	-30
	5.Computers (1Qv) ,##2-7,Tabl.4	3354	5.Computers (1Qv) ,##2-7,Tabl.4	3212	-142
	Total by L07				582
L08 23.02.04	1. N.Glavatska Tabl.3, #1	120	1. N.Glavatska Tabl.3, #1		+120
	2. Chemical analysis, Tabl. 7, # 11	0	2. Chemical analysis, Tabl.7, # 1	30	-30
23.02.02	3. Repairing/maintenance of equipment, Tabl.7,#8	60	3. Repairing/maintenance of an equipment, Tabl.7,#8	150	
	Total by L08				
L09 1.03.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L09 16.03.04	2. Special holder and device for diffractometer Tabl. 7, # 2	0	2. Special holder and divice for diffractometer, Tabl. 7, # 2		-100
	Total by L09				100
	Total 3Qv				1108
Redirection 4 Qv					
L11 16.06.04	1. N.Glavatska Tabl.3, #1	110	1. N.Glavatska Tabl.3, #1		+110
	2. Chemical analysis, Tabl. 7, # 9	0	2. Chemical analysis, Tabl. 7, p 11	30	-30
	3. Repairing/maintenance of equipment, Tabl.7,#6	70	3. Repairing/maintenance of a equipment, Tabl.7,#8	150	-80
	Total by L11				110
L12 17.06.04	1. G. Mogylnyy Tabl.3, #15	500	1. G. Mogylnyy Tabl.3, #15	600	-100
	2. V.Bliznyuk Tabl.3, #16	270	2. V.Bliznyuk Tabl.3, #16	216	+44
	3. A.Rudenko Tabl.3, #17	240	3. A.Rudenko Tabl.3, #17.	210	+30
	4. I.Urubkov Tabl.3, #18	180	4.I.Urubkov Tabl.3, #17	216	-36
	5. I.Surzhenko Tabl.3, #19	342	5. I.Surzhenko Tabl.3, #19	144	+198

	6. A.Urubkov Tabl.3, #20	375	6. A.Urubkov Tabl.3, #20	255	+120
	7. E.Bersudskyy Tabl.3, #23	90	7. E.Bersudskyy Tabl.3, #23	306	-216
	8. I.Glavatskyy Tabl.3, #13	560	8. I.Glavatskyy Tabl.3, #13	600	-40
	Total by L12				648
	Total 4 Qv				758
	Redirection 5 Qv				
L10 15.06.04	1. Travel to Institute Laue-Langevin ILL (Grenoble, France) for the neutron diffraction experiment	1150	1. Tabl.8,	0	+1150
	2. Travel to Berlin, Germany 4Qv #2,Tabl.8	190	2. Travel to Berlin, Germany, #2Tabl 8.	340	-150
	3. Travel for the EPDIC -9 conference, #1,Tabl.8	0	3. 3. Travel for the EPDIC -9 conference, #1,Tabl.8	1000	-1000
	Total by L10				1150
L13 17.06.04	1.Computers (Non-Capital) Tabl.4,# 1-7	5012	1.Computers (Non-Capital) Tabl.4,# 1-7	4354	+658
	2.. Portative Mechanical testing Machine, Tabl.4,# 1		2. Portative Mechanical testing Machine, Tabl.4,# 1	18000	-658
	Total by L13				658
L14 21.06.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L14 21.06.04	2. Repairing of a room Tabl.7,#11	0	2. Repairing of a room, Tabl.7,#11	100	-100
	Total by L14				100
L15 08.07.04	1. Travel to Cancun for Symposium on “Magnetic Shape Memory Alloys“, Tabl.8,	937		0	+937
	2. Travel to France for ESOMAT conference, Tabl.8 #5	63	2. Travel to France for ESOMAT conference, Tabl.8 #5	1000	-937
	Total by L15				937
L16 15.07.04	1. V.Gavruljuk (Tabl.3#1)	2790 1-5 Qv	1. V.Gavruljuk (Tabl.3#1)	5010 1-8 Qv	-2220
	2. V. Is’yanov (Tabl.3 #19)	2220 5-8 Qv	2. V. Is’yanov (Tabl.3, #19)	0 5-8 Qv	+2220
	3.E.Bersudskyy (Tabl 3#18)	0 4 Qv	3. 3.E.Bersudskyy (Tabl 3#18)	108 4 Qv	-108
	4.E.Bersudskyy (Tabl 3#18)	108 5 -6Qv	3. 3.E.Bersudskyy (Tabl 3#18)	0 5-6 Qv	+108
	Total by L16				2328
L17 01.09.04	1. I.Zasimchuk (Tabl.3#3)	400 5 Qv	1. I.Zasimchuk (Tabl.3#3)	500 5 Qv	-100
	2. Artem.Urubkov (Tabl.3 #15)	330 5 Qv	2. A.Urubkov (Tabl.3 #15)	240 5 Qv	+90
	3.I Surzenko (Tabl 3#14)	216 5 Qv	3. I Surzenko (Tabl 3#14)	144 5 Qv	+76
	4. Ilya Urubkov (Tabl.3 #15)	180 5 Qv	4. Ilya Urubkov (Tabl.3 #15)	216 5 Qv	-36

5.V.Gavriljuk (Tabl.3#2)	300 5 Qv	5.V.Gavriljuk (Tabl.3#2)	630 5 Qv	-330
6. V.Isyanov (Tabl.3#19, New participant)	300 5 Qv	6. V.Isyanov (Tabl.3#19)	0 5 Qv	+300
7. V.Cherepin (Tab3.5#5)	0 5Qv	7. V.Cherepin (Tab3.5#5)	250 5Qv	-250
8. V.Cherepin (Tab3.5#5)	250 6Qv	8. V.Cherepin (Tab3.5#5)	0 5Qv	+250
9. V.Uvarov (Tabl.3#11)	9	10. V.Uvarov (Tabl.3#11)	350 5 Qv	-175
10. V.Uvarov (Tabl.3#11)	175 7 Qv	10. V.Uvarov (Tabl.3#11)	0 7 Qv	+175
Total by L17				891
Total 5 Qv				5994

Redirection 6 Qu

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)
L19 22.10.04	1. Scanner (Non-Capital) Annex 1, Tabl.4,	100	1.Scanner (Non-Capital) Annex 1 Tabl.4	0	+100
L19 22.10.04	2. Fax Annex 1 (Non-Capital) Tabl.4	128	2. Fax, Annex 1 (Non-Capital) Tabl.4	0	+128
L19 22.10.04	3. Equipment, Annex 1, Capital, Table 4, #1.	2799 - 1913 (L18)-658 (L13) - 228 (L19) = 0	4. Equipment, Annex 1, Capital, Table 4, #1.	2799	-228
	Total by L19				228
L20 09.11.04	1. Mr.O.Rudenko Annex 1, Tabl.3 ,#12	990	1. . Mr.O.Rudenko Annex 1, Tabl.3, #12	1500	-510
L20 09.11.04	2. Mr.A.Urubkov Annex 1, Tabl.3, #15	2220	2. Mr.A.Urubkov Annex 1, Tabl.3, #15	2010	+210
L20 09.11.04	3. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2602	3. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2502	+100
L20 09.11.04	4.Mrs.I. Surzenko Annex 1, Tabl.3, #14	1532	4.Mrs.I. Surzenko Annex 1, Tabl.3, #14	1332	+200
	Total by L20				510
L20 09.11.04			1. Mr.A.Urubkov Annex 1, Tabl.3, #15	2220	
L21 09.11.04	1. Mr.A.Urubkov Annex 1, Tabl.3, #15	1665			-555
L20 09.11.04			2. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2602	
L21 01.12.04	2. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2807			+205

L21 01.12.04	3. Mr.I.Glavatskiy Annex 1, Tabl.3, #8	4900	3. Mr.I.Glavatskiy Annex 1, Tabl.3, #8	4800	+100
L21 01.12.04	4. Mr. I.Urubkov Annex 1, Tabl.3, #13	1656	4. Mr. I.Urubkov Annex 1, Tabl.3, #13	1476	+180
L21 01.12.04	5.Dr N.Glavatska Annex 1, Tabl.3, #1	13090	4.Dr N.Glavatska Annex 1, Tabl.3, #1	13020	+70
	Total by L21				555
L18 10.09.04	1. Flexi Force (Non-Capital) Tabl.4	163	1. Flexi Force (Non-Capital) Tabl.4,	0	+163
	2. Eguipment for chemical cutting of samples “Struna” (Non-Capital) Tabl.4	1750	2. Eguipment for chemical cutting of samples “Struna” (Non-Capital) Tabl.4 #4	0	+1750
	3. Portative mechanical testing machine Tabl.4, #1 (Capital)	16087	3 Portative mechanical testing machine Tabl.4, #1	18000	-1913
	Total by L18				1913
	Total 6 Qu				3206

6. Delays and suggestions.

Studies are performed in accordance with the project plan. The diamont cutting disc for the cutting mashine MINITOM is distroyed. We have problems to cut the oriented single crystal specimens for the magneic field induced strain measurement. We need extremly to bay a new ones. We will send the corresponding letter with details of redirections costs we ask about.

N.Glavatska

Project Manager

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

Project manager: Glavatska Nadiya Ivanivna, Senior Scientists Researcher
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Institutions: Institute for Metal Physics
Financing parties: USA, European Office of Aerospace Research & Development (EOARD)
Operative commencement date: 1 July 2004
Project duration: 2 years
Date of submission: 25 April 2005

	Content of the quarterly progress report for quarter <04>	PAGE 1

1. Summary of progress.

Stage number and title	# 4 Design the high – temperature magnetic shape memory actuating elements from searched alloys and study their thermo-mechanical stability

Actual progress

According to the project plan, studies were directed on the clarification of the possibility to obtain the magnetic field induced strain in new high temperature Ni-Mn-Ga and alloyed Ni-Mn-Ga-(X) compositions as well as on investigation they're thermal and mechanical stability. Basing on the alloying effect studied in the previous quarter, Ni-Mn-Ga-Cu and Ni-Mn-Ga-Fe compositions, having optimal relation between Curie and martensitic transformation temperatures, were selected for melting of new alloys and followed study. These alloys were selected taking into account potential price of new alloys because change of the very expensive Ga by Fe or Cu can cause decrease of the final price of magnetic shape actuators, if these alloys can produce magnetic field induced strain.

Ni-Mn-Ga and Ni-Mn-Ga-Cu polycrystals were melted. Single crystals with weight 30-90 g were grown using polycrystals (#4.1). Homogenization and treatments for ordering followed were used thereafter. Chemical analysis of new single crystal was done. Table 1 shows the chemical content of new single crystals. The single crystal №1 (Tabl.1) has grown in the previous quarter. We studied change in the treatment condition on the phase content and structure of this Fe-alloyed single crystal (#4.1).

Study of phase content of the Ni-Mn-Ga-Cu and Ni-Mn-Ga-Fe single crystals was done using x-ray diffraction. Used changes in the treatment (time of ordering and the cooling rate) of Fe-alloyed crystal caused disappearance of the second phase.

Phase transformation (both structural and magnetic) temperatures were studied (Table 1) as well as temperature stability of martensite phase in the range from room temperature up to the that of the martensite-austenite transformation A_S (#4.3).

Table 1. Chemical compositions (at. %) and temperatures of phase transformations of the new single crystals (^{0}C).

N	Ni	Mn	Ga	Fe	Cu	T_c	M_S	M_f,	A_s	A_f
1	52,24	20,52	20,19	6,97	-	115	85.7	78.8	88	100
2	53,04	23,94	22,95	0,04	0,01	106	97	94	*	*
3.1	50,2	25,5	22,87	-	1,43	86	32	33	35	38
3.2	49,66	27,85	20,74	-	1,7	104	48	45	56	60

* to be rechecked

Single crystal growth techniques are optimized to improve the quality of the crystals (#4.3). To improve the quality of Cu-alloyed single crystals during casting we applied the slow cooling regime (12-24 hours). This led to higher Mn loss, affecting the Ni-Mn-Ga and Cu ratio, consequently resulting in lower martensite transformation temperature M_S (Table 1). This result points the necessity of pre-casting compositions corrections in the way of increased Mn concentration.

Crystal structure of the martensite in developed single crystals was investigated. Alloys with Cu (№3.1 and №3.2, Table 1) possess 5-layered martensite structure, while Fe-alloyed crystals (№1, Table 1) have 7-layered crystal structure of martensite, after applied optimized thermal treatments. Alloy №2 has non-modulated tetragonal martensite crystal structure in the studied temperature range. As it was shown in the preceding quarters, alloys with non-modulated tetragonal martensites do not strain in the magnetic field up to that of the saturation of magnetization. At the same time, as it we discovered that type of martensite lattice possesses giant mechanical super-elasticity at room temperature and above. Single crystals of the alloy №2, with tetragonal non-modulated lattice of martensite, were cast for studies of the linear mechanical super-elasticity and thermal shape memory effect in wide range of mechanical stresses (#4).

Searching for the optimal single crystal growth regimes is continued, aiming to improved crystal quality (#4.2). Optimization of the crystal growth regime were performed for the Ni-Mn-Ga and Ni-Mn-Ga-Fe alloys, that were cast and studied in the 7th and previous quarters, since, as we found in the current quarter, quality of the single crystal is crucial for the magnetic field induced strains (#4.2). Column-type growth leads to high brittleness of single crystals, and thus to their fast destruction during thermal treatment, cycling and investigations (#4.4). Optimization of the single crystal growth for Ni-Mn-Ga-Fe and Ni-Mn-Ga-Cu requires special studies.

Electronic structure of Cu-alloyed crystals was studied experimentally in martensite and austenite phases (Table 1, 3.1) (#4.8). Yet the experiment is not finished due to X-ray fluorescent spectrometer breakdown. It will be resumed after reconstruction of the instrument.

According to the project work plan, the temperature stability of magnetic field induced strains (MFIS) was studied (# 4.2, 4.3). Preliminary results obtained indicate less MFIS stability at raised temperatures ($T>50^0$C), close to temperatures of martensite-austenite transformation in alloys with 7-layered martensite lattice. Experimental studies shows that obtained MFIS are decreasing with time after magnetic field switch-off.

To clarify the obtained results of temperature dependence on MFIS we provided theoretical investigations, concerning the temperature influence on the twinned structure of martensite (# 4.9, 4.3), also involving the temperature fluctuations of microstresses. The theoretical basis for the effect of thermal fluctuations of microstresses on stability of ferromagnetic martensites were developed in the frames of the project and was published this year: V. L'vov, O. Rudenko, N. Glavatska, Physical review B **71**, 024421 (2005). Investigations are also build upon the statistical approach on the martensite twin reorientation (Glavatska N. I., Rudenko A. A., Glavatskiy I. N., L'vov V. A., Statistical model of magnetostrain effect in martensite. JMMM, **265**, 142 (2003). Theoretical model for the mechanical and magnetic induced stresses fluctuations has been developed also (#4.9, 4.7). The role of the thermal phonons on the crystals with cubic lattice of austenite phase. At first the fluctuating strain in crystal were studied. It was shown, that fluctuating strains has stronger temperature dependence compared to those of the elastic stresses. According to the model being developed, thermal stability as well as intensity of the magneto-elastic (which results to the magneto-plastic) strains depends on the martensite twin platelets width. This way it is shown that if martensitic twin platelets width increases 3 times, the resulting intensity of the thermal strain fluctuations raises eight times. This result predicts different temperature dependence and thermal stability of MFIS within the different types of martensite crystal lattice. Model development and completion, together with article preparation would be continued in the 8^{th} quarter.

As a continuation of the research performed according to the project plan in the field of theory creation for magnetoplastic ferromagnetic martensites, we made an attempt to develop theory of that phenomenon from the basic principles of magnetoelasticity: article V. L'vov "Spin-lattice effects in the Ni-Mn-Ga shape- memory alloys" was submitted for publication.

Also preliminary search for the possibility of patent application concerned the results of magnetic field induced strains at increased temperatures was performed. Patent application concerning with the giant supeelasticity we have found is continued.

Additionally, the upgrade and maintenance was provided for the automatic mechanical loading system for magnetic dilatometer.

2. Summary of personnel commitment.

Following participants were involved in study in accordance with sub-stages #4.1, 4.6: N. Glavatska, I.Glavatskiy (choice of composition of polycrystals,) E.Tarusin (heat treatments). I. Zasimchuk and L. Matvienko (grown single crystals and optimized the grown routines), I. Glavatskyy and A. Dobrinskiy (determination of phase transformation temperatures by the dilatometry and with low-field magnetic susceptibility methods. I.Glavatskiy measured magnetic field induced strain (# 4.3). V. Lvov together with N.Glavatska performed theoretical analysis of temperature dependence the detwinning effect and magnetic field induced strain and its thermal stability (# 4.9, 4.3, 4,7). I.Surshenko and N/Zaitzeva studied crystal structure and performed the phase analysis of policrystals using x-ray diffraction method. I.Surzenko also performed together withG.Mogylnyy orientation analysis of single crystals using x-ray texture method (#4.1). Mechanical elasticity and plasticity studied I.Glavatskiy (#4.5). V.Uvarov and I.Urubkov studied preliminary the electronic structure of Ni-Mn-Ga-Cu) martensite (#4.8). M. Knysh performed the technical maintenance of equipment and made some required metal works. V. Isyanov headed by V.Cherepin made remaining of the loading system for the magnetic dilatometer and improved its construction. N.Glavatska analysed all results obtained and managed the project performance.

3. Description of travels.

We have no travels in 6 quarter.

4. Current status.

Scheduled works were performed according to the project work plan (stage 4). Main result of the stage is the obtained MFIS in single crystals of the new Ni-Mn-Ga-Cu and Ni-Mn-Ga-Fe ferromagnetic martensite alloys. Main results of the stage #4 concernson the new magnetic shape memory martensite we have found Ni-Mn-Ga-Cu magnetic field induced strain founded in this martensite at temperature 50^0C. Another important result concerns with the theoretical investigation of the temperature effect on detwinning of martensite under magnetic field /stress and magnetic field induced strain stability with temperature.

5. Problems encountered.

Project participant Mr. G.Mogylnyy was very busy with his PhD thesis preparation and planed to travel abroad for 1 month. Therefore we included for the project the new participant Dr. Nataliya Zaitzeva. Shi is senior scientists' researcher in IMP and specializes in the x-ray diffraction. Mrs. N.Zaitzeva will perform some experiments planned for Mr.G. Mogylnyy.

Table below explains details of the costs redirection.

Table. Redirection.

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)
	Redirection 1 Qv				
L01 27.08.03	1. Diamond Cuting disks Tabl.4, #.17	411	1. Diamond Cuting disks Tabl. #.17	160	+251
	4. Memory DIMM 32 Mb SDRAM. Annex 1, Tabl. 4, #	0	4 .Memory DIMM 32 Mb SDRAM Winchester, Tabl.4 #11	120	-120
L04 23.09.03	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	1000		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	0	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	700	-700
	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	0	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2		-120
	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	80	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	180	-180
	Total by 1Qv				1411
	Redirection 2 Qv				
L02 27.08.03	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder according to the project) Tabl.3, #.1.	150			+150
	2. Repairing/maintenance of equipment Tabl.7, # 6	0	2. Repairing/maintenance of equipment Tabl.7, # 6	150	-150
L03 27.08.03	1. N.Glavatska (Payment by cash for power supply temperature controller, Tabl.3, #.1	100			+100
	2. Power supply , Tabl. 7, # 20	0	2. Power supply for temperature controller Tabl. 7, # 20	100	-100
	2. Repairing/maintenance of equipment #6 Table 7	84	Repairing/maintenance of equipment #6 Table 7	150	-66
	Total 2 Qv				$316
Redirection 3 Qv					
L06 23.09.03	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1506	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1200	+306
	2. Travel to Berlin, Germany 2Qv #2,Tabl.8	0	2. Travel to Berlin, Germany, #2Tabl.	220	-220
	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	64	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	150	-86
	Total L06				306
L07 19.02.04	1. Adapter and Step down ring for optical microskope	582	1. Adapter and Step down ring for optical microskope	0	+582

	#21, Tabl.4		#21, Tabl.4		
	2. Stabilisator of voltage #14, Tabl. 4	0	2. Stabilisator of voltage #14, Tabl. 4	355	-355
	3. Communication (1-3Qv) #5,Tabl.7	0	3. Communication (1-3Qv) #5,Tabl.7	55	-55
	4. Chemical analysis (1Qv),#5,Tabl.7	0	4. Chemical analysis composition,(1Qv),#5,Tabl.	30	-30
	5.Computers (1Qv) ,##2-7,Tabl.4	3354	5.Computers (1Qv) ,##2-7,Tabl.4	3212	-142
	Total by L07				582
L08 23.02.04	1. N.Glavatska Tabl.3, #1	120	1. N.Glavatska Tabl.3, #1		+120
	2. Chemical analysis, Tabl. 7, # 11	0	2. Chemical analysis, Tabl.7, # 1	30	-30
23.02.02	3. Repairing/maintenance of equipment, Tabl.7,#8	60	3. Repairing/maintenance of an equipment, Tabl.7,#8	150	
	Total by L08				
L09 1.03.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L09 16.03.04	2. Special holder and device for diffractometer Tabl. 7, # 2	0	2. Special holder and divice for diffractometer, Tabl. 7, # 2		-100
	Total by L09				100
	Total 3Qv				1108
Redirection 4 Qv					
L11 16.06.04	1. N.Glavatska Tabl.3, #1	110	1. N.Glavatska Tabl.3, #1		+110
	2. Chemical analysis, Tabl. 7, # 9	0	2. Chemical analysis, Tabl. 7, p 11	30	-30
	3. Repairing/maintenance of equipment, Tabl.7,#6	70	3. Repairing/maintenance of a equipment, Tabl.7,#8	150	-80
	Total by L11				110
L12 17.06.04	1. G. Mogylnyy Tabl.3, #15	500	1. G. Mogylnyy Tabl.3, #15	600	-100
	2. V.Bliznyuk Tabl.3, #16	270	2. V.Bliznyuk Tabl.3, #16	216	+44
	3. A.Rudenko Tabl.3, #17	240	3. A.Rudenko Tabl.3, #17.	210	+30
	4. I.Urubkov Tabl.3, #18	180	4.I.Urubkov Tabl.3, #17	216	-36
	5. I.Surzhenko Tabl.3, #19	342	5. I.Surzhenko Tabl.3, #19	144	+198
	6. A.Urubkov Tabl.3, #20	375	6. A.Urubkov Tabl.3, #20	255	+120
	7. E.Bersudskyy Tabl.3, #23	90	7. E.Bersudskyy Tabl.3, #23	306	-216
	8. I.Glavatskyy Tabl.3, #13	560	8. I.Glavatskyy Tabl.3, #13	600	-40
	Total by L12				648
	Total 4 Qv				758
	Redirection 5 Qv				
L10 15.06.04	1. Travel to Institute Laue-Langevin ILL (Grenoble, France) for the neutron diffraction experiment	1150	1. Tabl.8,	0	+1150
	2. Travel to Berlin, Germany 4Qv #2,Tabl.8	190	2. Travel to Berlin, Germany, #2Tabl 8.	340	-150
	3. Travel for the EPDIC -9 conference, #1,Tabl.8	0	3. 3. Travel for the EPDIC -9 conference, #1,Tabl.8	1000	-1000
	Total by L10				1150
L13 17.06.04	1.Computers (Non-Capital) Tabl.4,# 1-7	5012	1.Computers (Non-Capital) Tabl.4,# 1-7	4354	+658
	2.. Portative Mechanical		2. Portative Mechanical testing	18000	-658

	testing Machine, Tabl.4,# 1		Machine, Tabl.4,# 1		
	Total by L13				658
L14 21.06.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L14 21.06.04	2. Repairing of a room Tabl.7,#11	0	2. Repairing of a room, Tabl.7,#11	100	-100
	Total by L14				100
L15 08.07.04	1. Travel to Cancun for Symposium on "Magnetic Shape Memory Alloys", Tabl.8,	937		0	+937
	2. Travel to France for ESOMAT conference, Tabl.8 #5	63	2. Travel to France for ESOMAT conference, Tabl.8 #5	1000	-937
	Total by L15				937
L16 15.07.04	1. V.Gavruljuk (Tabl.3#1)	2790 1-5 Qv	1. V.Gavruljuk (Tabl.3#1)	5010 1-8 Qv	-2220
	2. V. Is'yanov (Tabl.3 #19)	2220 5-8 Qv	2. V. Is'yanov (Tabl.3, #19)	0 5-8 Qv	+2220
	3.E.Bersudskyy (Tabl 3#18)	0 4 Qv	3. 3.E.Bersudskyy (Tabl 3#18)	108 4 Qv	-108
	4.E.Bersudskyy (Tabl 3#18)	108 5 -6Qv	3. 3.E.Bersudskyy (Tabl 3#18)	0 5-6 Qv	+108
	Total by L16				2328
L17 01.09.04	1. I.Zasimchuk (Tabl.3#3)	400 5 Qv	1. I.Zasimchuk (Tabl.3#3)	500 5 Qv	-100
	2. Artem.Urubkov (Tabl.3 #15)	330 5 Qv	2. A.Urubkov (Tabl.3 #15)	240 5 Qv	+90
	3.I Surzenko (Tabl 3#14)	216 5 Qv	3. I Surzenko (Tabl 3#14)	144 5 Qv	+76
	4. Ilya Urubkov (Tabl.3 #15)	180 5 Qv	4. Ilya Urubkov (Tabl.3 #15)	216 5 Qv	-36
	5.V.Gavriljuk (Tabl.3#2)	300 5 Qv	5.V.Gavriljuk (Tabl.3#2)	630 5 Qv	-330
	6. V.Isyanov (Tabl.3#19, New participant)	300 5 Qv	6. V.Isyanov (Tabl.3#19)	0 5 Qv	+300
	7. V.Cherepin (Tab3.5#5)	0 5Qv	7. V.Cherepin (Tab3.5#5)	250 5Qv	-250
	8. V.Cherepin (Tab3.5#5)	250 6Qv	8. V.Cherepin (Tab3.5#5)	0 5Qv	+250
	9. V.Uvarov (Tabl.3#11)	9	10. V.Uvarov (Tabl.3#11)	350 5 Qv	-175
	10. V.Uvarov (Tabl.3#11)	175 7 Qv	10. V.Uvarov (Tabl.3#11)	0 7 Qv	+175
	Total by L17				891
	Total 5 Qv				5994

Redirection 6 Qu

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)
L19 22.10.04	1. Scanner (Non-Capital) Annex 1, Tabl.4,	100	1.Scanner (Non-Capital) Annex 1 Tabl.4	0	+100
L19 22.10.04	2. Fax Annex 1 (Non-Capital) Tabl.4	128	2. Fax, Annex 1 (Non-Capital) Tabl.4	0	+128
L19 22.10.04	3. Equipment, Annex 1, Capital, Table 4, #1.	2799 - 1913 (L18)-658 (L13) - 228 (L19) = 0	4. Equipment, Annex 1, Capital, Table 4, #1.	2799	-228
	Total by L19				228
L20 09.11.04	1. Mr.O.Rudenko Annex 1, Tabl.3 ,#12	990	1. . Mr.O.Rudenko Annex 1, Tabl.3, #12	1500	-510
L20 09.11.04	2. Mr.A.Urubkov Annex 1, Tabl.3, #15	2220	2. Mr.A.Urubkov Annex 1, Tabl.3, #15	2010	+210
L20 09.11.04	3. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2602	3. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2502	+100
L20 09.11.04	4.Mrs.I. Surzenko Annex 1, Tabl.3, #14	1532	4.Mrs.I. Surzenko Annex 1, Tabl.3, #14	1332	+200
	Total by L20				510
L20 09.11.04			1. Mr.A.Urubkov Annex 1, Tabl.3, #15	2220	
L21 09.11.04	1. Mr.A.Urubkov Annex 1, Tabl.3, #15	1665			-555
L20 09.11.04			2. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2602	
L21 01.12.04	2. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2807			+205
L21 01.12.04	3. Mr.I.Glavatskiy Annex 1, Tabl.3, #8	4900	3. Mr.I.Glavatskiy Annex 1, Tabl.3, #8	4800	+100
L21 01.12.04	4. Mr. I.Urubkov Annex 1, Tabl.3, #13	1656	4. Mr. I.Urubkov Annex 1, Tabl.3, #13	1476	+180
L21 01.12.04	5.Dr N.Glavatska Annex 1, Tabl.3, #1	13090	4.Dr N.Glavatska Annex 1, Tabl.3, #1	13020	+70
	Total by L21				555
L18 10.09.04	1. Flexi Force (Non-Capital) Tabl.4	163	1. Flexi Force (Non-Capital) Tabl.4,	0	+163
	2. Eguipment for chemical cutting of samples "Struna" (Non-Capital) Tabl.4	1750	2. Egguipment for chemical cutting of samples "Struna" (Non-Capital) Tabl.4 #4	0	+1750
	3. Portative mechanical testing machine Tabl.4,	16087	3 Portative mechanical testing machine Tabl.4, #1	18000	-1913

#1 (Capital)	
Total by L18	1913
Total 6 Qu	3206

Redirection 7 Qu

Date	*Requested categories (new)*	*Requested cost, $ (new)*	*Original categories (old)*	*Estimated cost, $ (old)*	*Redirected cost, $ (new-old)*
L22 16.02.05	1. Mr.G.Mogylnyy Annex 1, Tabl.3, #10	3800	1. Mr.G.Mogylnyy Annex 1, Tabl.3, #10	4800	-1000
L22 16.02.05	2. Dr.N.Zaitzeva Annex 1, Tabl.3	1000	2. Dr.N.Zaitzeva Annex 1, Tabl.3, #	0	+1000
	Total 7 Qu				1000

6. Delays and suggestions.

Studies are performed in accordance with the project plan.

N.Glavatska

Project Manager

"High temperature magnetic shape memory Ni-Mn-Ga alloys for a new class of actuators and sensors"

Project manager: Glavatska Nadiya Ivanivna, Senior Scientists Researcher
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Institutions: Institute for Metal Physics
Financing parties: USA, European Office of Aerospace Research & Development (EOARD)
Operative commencement date: 1 July 2004
Project duration: 2 years
Date of submission: 25 July 2005

	Content of the quarterly progress report for quarter <04>	PAGE 1

1. Summary of progress.

Stage number and title	# 4 Design the high – temperature magnetic shape memory actuating elements from searched alloys and study their thermo-mechanical stability

Actual progress

In accordance to the stage assignment, main efforts were put on the obtaining the magnetic field induced strains under increased temperatures and investigation of the magnetic field induced strain stability. Main attention was paid to the investigation of the compositions alloyed with copper and iron, which were chosen to be most promising during the preceding quarters. Main result of the stage is the obtained large strains (4%) induced by the applied magnetic field of relatively small magnitude 0.2-0.3T at higher temperatures 50-58^{0}C, whish was the main practical task of the project.

From the corrected Ni-Mn-Ga-Cu and Ni-Mn-Ga-Fe compositions polycrystalline ingots were melt, that were used to grow the single crystals about 30g weight (#4.1). Single crystal growth was performed after the corrected scheme, which means slow growth rate and utilization of the single crystalline precipitate, to obtain the needed crystallographic orientation f the specimen.

For homogenization and ordering of the single crystalline ingots heat treatments procedures were applied (#4.1). Then, chemical analysis of the obtained single crystals was performed. It was found that slow single crystal growth rate causes considerable chemical inhomogeneity along axis of growth, resulting in the significant difference of temperatures of phase transformations (Table 1).

Thermal cycling, in the regimes used for non-alloyed specimens and adjusted by the results of investigations in the terms of the project, does not fully remove the chemical inhomogeneity (4.6) (Table 1).

Table 1. Chemical inhomogeneity of the single crystal (chemical composition - at %, temperature - K)

N	Ni	Mn	Ga	Fe	Ms	Mf	As	Af	Tc
NMG10 top	48,4	29,23	22,3	0,07	301	274,5	280	303	371,5
NMG10 bottom	48,86	28,66	22,43	0,05	299	277	282	303	373
N11top	49,63	23,45	21,56	5,36	314	299	302	320	399
N11 central	50,86	20,25	23,74	5,15	279,5	275	279	286	401

Slower rate of the single crystal growth leads to the better quality of the crystals (# 4.2), though at the same time brings to the deviation of the chemical composition from the expected one, being calculated during the initial furnace feed preparation (including the Mn loss due to evaporation). This proves the necessity of the additional systematic studies of the influence of heat treatment on chemical composition of the doped alloys. Though these systematic investigations are beyond the terms of the current project. Existence of such chemical inhomogeneities was clearly shown by the new electrochemical cutting method for the single crystals. Feature of the developed method allows visualization of the existing chemical inhomogeneities and determination of their dimensions. All necessary documents for patenting the developed method are being prepared.

Temperatures of the structural and magnetic phase transformations of the new single crystals were determined. X-ray investigation of the phase composition of single crystals and their orientation analyses were conducted, after that single crystalline specimens were cut and prepared for the thermo-magneto-mechanical treatment to obtain magnetic field induced strains (#4.1).

During investigations of the temperature dependence of the crystal lattice parameters by means of neutron diffraction experiments (BENSC, Berlin), our previously announced existence of the additional magnetic order transition at low temperatures in martensite phase. Temperature dependence of the crystal lattice parameters of the new doped Ni-Mn-Ga alloy in the temperature interval of the martensite existence.

Magnetic field induced strains in new ferromagnetic martensitic alloys of Ni-Mn-Ga-Fe and Ni-Mn-Ga-Cu, at high temperatures (58^0C) were obtained and studied (# 4.2). It is shown that maximal magnitude of the magnetic field induced strains, determined by the crystal lattice parameters, decreases according to their strong temperature dependence.

By the results of the neutron diffraction studies (HMI, Berlin and Grenoble, ILL - July 2004) the crystallographic affiliation of the 5-layered martensite, possessing magnetic shape memory effect was corrected. It was shown that this type of martensite belongs to the monoclinic syngony with P2/m space group. Crystal lattice parameters were defined more accurately.

For the first time were made theoretical computations of the electronic structure for the 5-layered monoclinic martensite of Ni_2MnGa alloy (for the temperatures of 300K, 220K and 200K) according to the new crystallographic data. Until this time in the literature, real 5-layered martensite unit cell were approximated by the simple tetragonal lattice, especially in all of the electronic structure calculations. Also, computations of the electronic structure of the high-ordered martensite phase for the alloy doped with iron (5%) and copper (5% and 10%) were performed. Computations of the local magnetic moments of all non-equivalent atoms were made, showing that doping affects only the close neighbors of the substitution atoms. Magnetic moments and charges inside the MT-spheres of Ni, Mn, Ga atoms of the FCC, BCT and 5R phases of Ni_2MnGa alloy were compared (#4.1).

The development of the theoretical model for the effect of the thermal fluctuations on magneto-mechanical behavior and magnetization of ferromagnetic martensites possessing magnetic shape memory effect in the terms of the temperature stability investigations (# 4.3, 4.9) was finished. The article describing the theory is prepared and submitted for publication.

Continuing the study of the linear superelasticity in Ni-Mn-Ga and doped alloys (#4.5) we obtained giant magnitudes of the linear superelasticity (12%) at room temperature in iron- doped alloy. It is justified that value of the linear superelasticity depends on the loading speed.

The results obtained in the project are now summarized. By the main project results publications and two patents are being prepared (#4.11).

2. Summary of personnel commitment.

In the sub-stages #4.1, #4.6 took part: N. Glavatska, I.Glavatskyy (selection of compositions, regimes of polycrystal melting and heat treatments), E. Tarusin (heat treatments), I.Zasimchuk and L.Matvienko (single crystal growth). A.Dobrinsky performed measurements of phase transformation temperatures. Magnetic field induced strains was investigated by I.Glavatskyy (#4.3). Theoretical analysis of the temperature stability of magnetic field induced deformations was conducted by V.Lvov and N.Glavatska. They also developed the theory of fluctuating deformations, affecting the time- dependent behavior of martensite in the steady magnetic field or mechanical stress (# 4.9, 4.3, 4.7). X-ray phase analysis of the new poly- and single- crystals were performed by I.Surzhenko and N.Zaytseva. N.Zaytseva conducted investigations of the chemical inhomogeneities of single crystals by means of optical methods as well, in single crystalline specimens prepared by new electrochemical cutting method. N.Zaytseva also searched for the electrolyte and reactives for the new electrochemical cutting of the single crystals. I.Surzhenko together with G.Moghylny performed orientational analysis of the crystals by X-ray texture analysis method (#4.1). Mechanical properties and superelasticity were studied by I.Glavatskyy (#4.5). Electronic structure investigations of the iron-doped alloys (#4.8) were done by I.Urubkov and V.M.Uvarov. Electronic structure computations of the 5-layered martensites of Ni-Mn- Ga, Ni-Mn-Ga-Fe and Ni-Mn-Ga-Cu were conducted by I.Glavatskyy and I.Urubkov. M.Knysh performed needed metal works and preliminary specimen preparation. Under guidance of V.Cherepin, V.Isyanov provided maintenance and upgrade of the dilatometer temperature control system. N.Glavatska carried out the scientific guidance, co-ordination of the work and analysis of the obtained results by all the tasks of the project.

3. Description of travels.

I.Glavatskyy and I.Urubkov took the mission to the BENSC (Berlin) to provide neutron diffraction studies. Missions were reported.

Scheduled trip of the Prof. V.Lvov to Warsaw (Poland) for E-MRS conference participation with oral contribution in the September 2005 and trip of the N.Glavatska to the Partenit (Ukraine) to participate the ICFM conference (International Conference on the Functional Materials) with lecture, 2-8 October 2005. Assignments not reported yet.

4. Current status.

Scheduled works were performed according to the project work-plan (stage 4). Main result of the stage is the obtained magnetic field induced strains in new ferromagnetic martensites Ni-Mn-Ga-Fe and Ni-Mn-Ga-Cu at raised temperatures (58^0C), determination of the correct crystallography of martensite with 5-layred modulated structure. At the first time computed and theoretically investigated the electronic structure of the 5-layered monoclinic phase of Ni_2MnGa (for 300K, 220K and 200K). Until that, in literature, real unit cell of the 5-layered martensite were approximated by simple tetragonal lattice in electronic structure calculations.

5. Problems encountered.

Combined printer-scanner-copier-fax hp LaserJet 3015 (L19) was purchased, paid money for the alarm system setup (L24). Purchased DVD-RW+RW for information backup and storage (L26).

Made prepayments for the Prof. V.Lvov assignment to Warsaw (Poland) for E-MRS-2005 (symposium "Shape memory for Smart Materials") conference participation and assignment of N.Glavatska to participate with lecture in ICFM-2005 conference (Partenit, Ukraine) (L25, L26).

Some job redistribution between project participants were made, according to the top-priority needs in project tasks accomplishment – between I.Urubkov, V.Uvarov, I.Surzhenko and A.Dobrinsky (L26).

Details of the costs redirection are provided in table below.

Table. Redirection.

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)
	Redirection 1 Qv				
L01 27.08.03	1. Diamond Cuting disks Tabl.4, #.17	411	1. Diamond Cuting disks Tabl. #.17	160	+251
	4. Memory DIMM 32 Mb SDRAM. Annex 1, Tabl. 4, #	0	4 .Memory DIMM 32 Mb SDRAM Winchester, Tabl.4 #11	120	-120
L04 23.09.03	1. Travel to Mexico for SMCr-2003 crystallography congress , Tabl.8,	1000		0	+1000
	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	0	2. Travel to Partenit Crimea for ISFD conference, Tabl.8 #1	700	-700
	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	0	3. Travel to Sanct-Petersburg, Russia, Tabl.8 #2	120	-120
	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	80	4. Travel to Charkiv, Physical -Technical Institute, Tabl.8 #3	180	-180
	Total by 1Qv				1411
	Redirection 2 Qv				
L02 27.08.03	3. N.Glavatska (Payment by cash for repairing of the goniometer and special holder according to the project) Tabl.3, #.1.	150			+150
	2. Repairing/maintenance of equipment Tabl.7, # 6	0	2. Repairing/maintenance of equipment Tabl.7, # 6	150	-150
L03 27.08.03	1. N.Glavatska (Payment by cash for power supply temperature controller, Tabl.3, #.1	100			+100
	2. Power supply , Tabl. 7, # 20	0	2. Power supply for temperature controller Tabl. 7, # 20	100	-100
	2. Repairing/maintenance of equipment #6 Table 7	84	Repairing/maintenance of equipment #6 Table 7	150	-66
	Total 2 Qv				$316
Redirection 3 Qv					
L06 23.09.03	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1506	1. Workshop "Interplay of Magnetism and Structure in Functional Materials" in Benasque (Spain), #3, Tabl.8,	1200	+306
	2. Travel to Berlin, Germany 2Qv #2,Tabl.8	0	2. Travel to Berlin, Germany, #2Tabl.	220	-220
	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	64	3. Repairing/maintenance of equipment (1Qv) #6,Tabl.7	150	-86
	Total L06				306
L07 19.02.04	1. Adapter and Step down ring for optical microskope #21, Tabl.4	582	1. Adapter and Step down ring for optical microskope #21, Tabl.4	0	+582

	2. Stabilisator of voltage #14, Tabl. 4	0	2. Stabilisator of voltage #14, Tabl. 4	355	-355
	3. Communication (1-3Qv) #5,Tabl.7	0	3. Communication (1-3Qv) #5,Tabl.7	55	-55
	4. Chemical analysis (1Qv),#5,Tabl.7	0	4. Chemical analysis composition,(1Qv),#5,Tabl.	30	-30
	5.Computers (1Qv) ,##2-7,Tabl.4	3354	5.Computers (1Qv) ,##2-7,Tabl.4	3212	-142
	Total by L07				582
L08 23.02.04	1. N.Glavatska Tabl.3, #1	120	1. N.Glavatska Tabl.3, #1		+120
L08 23.02.02	2. Chemical analysis, Tabl. 7, # 11	0	2. Chemical analysis, Tabl.7, # 1	30	-30
	3. Repairing/maintenance of equipment, Tabl.7,#8	60	3. Repairing/maintenance of an equipment, Tabl.7,#8	150	-90
	Total by L08				120
L09 1.03.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L09 16.03.04	2. Special holder and device for diffractometer Tabl. 7, # 2	0	2. Special holder and divice for diffractometer, Tabl. 7, # 2		-100
	Total by L09				100
	Total 3Qv				1108
Redirection 4 Qv					
L11 16.06.04	1. N.Glavatska Tabl.3, #1	110	1. N.Glavatska Tabl.3, #1		+110
	2. Chemical analysis, Tabl. 7, # 9	0	2. Chemical analysis, Tabl. 7, p 11	30	-30
	3. Repairing/maintenance of equipment, Tabl.7,#6	70	3. Repairing/maintenance of a equipment, Tabl.7,#8	150	-80
	Total by L11				110
L12 17.06.04	1. G. Mogylnyy Tabl.3, #15	500	1. G. Mogylnyy Tabl.3, #15	600	-100
	2. V.Bliznyuk Tabl.3, #16	270	2. V.Bliznyuk Tabl.3, #16	216	+44
	3. A.Rudenko Tabl.3, #17	240	3. A.Rudenko Tabl.3, #17.	210	+30
	4. I.Urubkov Tabl.3, #18	180	4.I.Urubkov Tabl.3, #17	216	-36
	5. I.Surzhenko Tabl.3, #19	342	5. I.Surzhenko Tabl.3, #19	144	+198
	6. A.Urubkov Tabl.3, #20	375	6. A.Urubkov Tabl.3, #20	255	+120
	7. E.Bersudskyy Tabl.3, #23	90	7. E.Bersudskyy Tabl.3, #23	306	-216
	8. I.Glavatskyy Tabl.3, #13	560	8. I.Glavatskyy Tabl.3, #13	600	-40
	Total by L12				648
	Total 4 Qv				758
	Redirection 5 Qv				
L10 15.06.04	1. Travel to Institute Laue-Langevin ILL (Grenoble, France) for the neutron diffraction experiment	1150	1. Tabl.8,	0	+1150
	2. Travel to Berlin, Germany 4Qv #2,Tabl.8	190	2. Travel to Berlin, Germany, #2Tabl 8.	340	-150
	3. Travel for the EPDIC -9 conference, #1,Tabl.8	0	3. 3. Travel for the EPDIC -9 conference, #1,Tabl.8	1000	-1000
	Total by L10				1150
L13 17.06.04	1.Computers (Non-Capital) Tabl.4,# 1-7	5012	1.Computers (Non-Capital) Tabl.4,# 1-7	4354	+658
	2.. Portative Mechanical testing Machine, Tabl.4,# 1		2. Portative Mechanical testing Machine, Tabl.4,# 1	18000	-658

	Total by L13				658
L14 21.06.04	1. N.Glavatska Tabl.3, #1	100	1. N.Glavatska Tabl.3, #1		+100
L14 21.06.04	2. Repairing of a room Tabl.7,#11	0	2. Repairing of a room, Tabl.7,#11	100	-100
	Total by L14				100
L15 08.07.04	1. Travel to Cancun for Symposium on "Magnetic Shape Memory Alloys", Tabl.8,	937		0	+937
	2. Travel to France for ESOMAT conference, Tabl.8 #5	63	2. Travel to France for ESOMAT conference, Tabl.8 #5	1000	-937
	Total by L15				937
L16 15.07.04	1. V.Gavruljuk (Tabl.3#1)	2790 1-5 Qv	1. V.Gavruljuk (Tabl.3#1)	5010 1-8 Qv	-2220
	2. V. Is'yanov (Tabl.3 #19)	2220 5-8 Qv	2. V. Is'yanov (Tabl.3, #19)	0 5-8 Qv	+2220
	3.E.Bersudskyy (Tabl 3#18)	0 4 Qv	3. 3.E.Bersudskyy (Tabl 3#18)	108 4 Qv	-108
	4.E.Bersudskyy (Tabl 3#18)	108 5 -6Qv	3. 3.E.Bersudskyy (Tabl 3#18)	0 5-6 Qv	+108
	Total by L16				2328
L17 01.09.04	1. I.Zasimchuk (Tabl.3#3)	400 5 Qv	1. I.Zasimchuk (Tabl.3#3)	500 5 Qv	-100
	2. Artem.Urubkov (Tabl.3 #15)	330 5 Qv	2. A.Urubkov (Tabl.3 #15)	240 5 Qv	+90
	3.I Surzenko (Tabl 3#14)	216 5 Qv	3. I Surzenko (Tabl 3#14)	144 5 Qv	+76
	4. Ilya Urubkov (Tabl.3 #15)	180 5 Qv	4. Ilya Urubkov (Tabl.3 #15)	216 5 Qv	-36
	5.V.Gavriljuk (Tabl.3#2)	300 5 Qv	5.V.Gavriljuk (Tabl.3#2)	630 5 Qv	-330
	6. V.Isyanov (Tabl.3#19, New participant)	300 5 Qv	6. V.Isyanov (Tabl.3#19)	0 5 Qv	+300
	7. V.Cherepin (Tab3.5#5)	0 5Qv	7. V.Cherepin (Tab3.5#5)	250 5Qv	-250
	8. V.Cherepin (Tab3.5#5)	250 6Qv	8. V.Cherepin (Tab3.5#5)	0 5Qv	+250
	9. V.Uvarov (Tabl.3#11)	9	10. V.Uvarov (Tabl.3#11)	350 5 Qv	-175
	10. V.Uvarov (Tabl.3#11)	175 7 Qv	10. V.Uvarov (Tabl.3#11)	0 7 Qv	+175
	Total by L17				891
	Total 5 Qv				5994

Redirection 6 Qu

Date	Requested categories (new)	Requested cost, $ (new)	Original categories (old)	Estimated cost, $ (old)	Redirected cost, $ (new-old)

L19 22.10.04	1. Scanner (Non-Capital) Annex 1, Tabl.4,	100	1.Scanner (Non-Capital) Annex 1 Tabl.4	0	+100
L19 22.10.04	2. Fax Annex 1 (Non-Capital) Tabl.4	128	2. Fax, Annex 1 (Non-Capital) Tabl.4	0	+128
L19 22.10.04	3. Equipment, Annex 1, Capital, Table 4, #1.	2799 - 1913 (L18)-658 (L13) - 228 (L19) = 0	4. Equipment, Annex 1, Capital, Table 4, #1.	2799	-228
	Total by L19				228
L20 09.11.04	1. Mr.O.Rudenko Annex 1, Tabl.3 ,#12	990	1. . Mr.O.Rudenko Annex 1, Tabl.3, #12	1500	-510
L20 09.11.04	2. Mr.A.Urubkov Annex 1, Tabl.3, #15	2220	2. Mr.A.Urubkov Annex 1, Tabl.3, #15	2010	+210
L20 09.11.04	3. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2602	3. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2502	+100
L20 09.11.04	4.Mrs.I. Surzenko Annex 1, Tabl.3, #14	1532	4.Mrs.I. Surzenko Annex 1, Tabl.3, #14	1332	+200
	Total by L20				510
L20 09.11.04			1. Mr.A.Urubkov Annex 1, Tabl.3, #15	2220	
L21 09.11.04	1. Mr.A.Urubkov Annex 1, Tabl.3, #15	1665			-555
L20 09.11.04			2. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2602	
L21 01.12.04	2. Mr.A.Dobrinskiy Annex 1, Tabl.3, #9	2807			+205
L21 01.12.04	3. Mr.I.Glavatskiy Annex 1, Tabl.3, #8	4900	3. Mr.I.Glavatskiy Annex 1, Tabl.3, #8	4800	+100
L21 01.12.04	4. Mr. I.Urubkov Annex 1, Tabl.3, #13	1656	4. Mr. I.Urubkov Annex 1, Tabl.3, #13	1476	+180
L21 01.12.04	5.Dr N.Glavatska Annex 1, Tabl.3, #1	13090	4.Dr N.Glavatska Annex 1, Tabl.3, #1	13020	+70
	Total by L21				555
L18 10.09.04	1. Flexi Force (Non-Capital) Tabl.4	163	1. Flexi Force (Non-Capital) Tabl.4,	0	+163
	2. Eguipment for chemical cutting of samples "Struna" (Non-Capital) Tabl.4	1750	2. Eguipment for chemical cutting of samples "Struna" (Non-Capital) Tabl.4 #4	0	+1750
	3. Portative mechanical testing machine Tabl.4, #1 (Capital)	16087	3 Portative mechanical testing machine Tabl.4, #1	18000	-1913
	Total by L18				1913
	Total 6 Qu				3206

Redirection 7 Qu

Date	*Requested categories (new)*	*Requested cost, $ (new)*	*Original categories (old)*	*Estimated cost, $ (old)*	*Redirected cost, $ (new-old)*
L22 16.02.05	1. Mr.G.Mogylnyy Annex 1, Tabl.3, #10	3800	1. Mr.G.Mogylnyy Annex 1, Tabl.3, #10	4800	-1000
L22 16.02.05	2. Dr.N.Zaitzeva Annex 1, Tabl.3	1000	2. Dr.N.Zaitzeva Annex 1, Tabl.3, #	0	+1000
	Total 7 Qu				1000

Redirection 8 Qu

Date	**Requested categories (new)**	**Requested cost, $ (new)**	**Original categories (old)**	**Estimated cost, $ (old)**	**Redirected cost, $ (new-old)**
L19 22.10.04	1. Scanner (Non-Capital) Annex 1, Tabl.4,	100	1.Scanner (Non-Capital) Annex 1 Tabl.4	0	+100
	2. Fax Annex 1 (Non-Capital) Tabl.4	128	2. Fax, Annex 1 (Non-Capital) Tabl.4	0	+128
	3. Equipment, Annex 1, Capital, Table 4, #1.	{18000-1913 (L18)-658 (L13)} - **228** (L19) =**15201**	4. Equipment, Annex 1, Capital, Table 4, #1.	18000	-228
	Total by L19				228
L24 21.04.05	1. Security of equipement (Annex 1 Tabl .7, #.1	474	1. 1. Security of equipement (, Annex 1 Tabl7, #.1	300	+174
L24 21.04.05	2 Repairing/maintenance of equipment (Annex 1Tabl.7, #.6	1026	2 Repairing/maintenance of equipment, (Annex 1Tabl. 7, #.6	1200	-174
Total by L24					174
L25 06.06.05	1 Travel to China, Shanghai), Annex 1Tabl.8, #.6, and L23 21.02.05	0	1 Travel to China, Shanghai), Annex 1Tabl.8, #.6, and L23 21.02.05	1026	-1026
L25 06.06.05	2. Travel to Poland)Annex 1Tabl.8, #.7,)	643	2. . Travel to Poland)Annex 1Tabl.8, #.7,)	0	+643
L25 06.06.05	3. Travel to Crimea (Annex 1Tabl.8, #.8)	383	*3. Travel to Crimea (Annex 1Tabl.8, #.8)*	0	+383
Total by L25					1026
L26 13.06.05	1. Diamond Cuting disks, L22 *16.02.05*	0	1. Diamond Cuting disks L22 16.02.05	*355*	-355
L26	2. Travel to Poland by	978	2.. Travel to Poland)	643	+335

13.06.05	V.L'vov (Annex 1Tabl.8, #.7, L25 06.06.05		Annex 1Tabl.8, #.7, L25 06.06.05)		
L26 13.06.05	3. Communication (Internet, Phone, Post) Annex 1Tabl.7, #.5	36	3. Communication (Internet, Phone, Post) Annex 1Tabl.7, #.5	180	-144
L26 *13.06.05*	4. Travel to Crimea (Annex 1Tabl.8, #.8, L25 06.06.05)	483	*4 Travel to Crimea (Annex 1Tabl.8, #.8, L25 06.06.05)*	383	+100
L26 *13.06.05*	*5. DVD-RW+RW ASUS (Annex 1Tabl.4, #.20*	64	*5. DvD-RW+RW ASUS (Annex 1Tabl.4, #.20*	0	+64
L26 *13.06.05*	*6.Pof.. V.L'vov Annex 1, Tabl.3, #7)*	4020	*.Pof.. V.L'vov (Annex 1, Tabl.3, #7)*	4343	+323
L26 *13.06.05*	*6.Other Direct Costs (Annex 1Tabl.7)*	2523	*6. Other Direct Costs (Annex 1Tabl.7)*	2846	-323
L26 *13.06.05*	*7. Mr. I.Urubkov (Annex 1, Tabl.3, #13, and L21)*	1656	*7. Mr. I.Urubkov Annex 1, Tabl.3, #13, L21)*	2106	+450
L26 *13.06.05*	*8 Prof.. V.Uvarov Annex 1, Tabl.3, #6)*	2000	*8 Prof.. V.Uvarov Annex 1, Tabl.3, #6)*	1550	-450
L26 *13.06.05*	*9. Mr. A.Dobrinskiy (Annex 1, Tabl.3, #13, and L21)*	2807	*9. Mr. A.Dobrinskiy (Annex 1, Tabl.3, #13, and L21)*	2557	-250
L26 *13.06.05*	*10. Mrs. I Surzhenko (Annex 1, Tabl.3, #14, and L20)*	1782	*10. Mrs. I Surzhenko (Annex 1, Tabl.3, #14, and L20)*	2030	+250
Total by L26					*1522*
	Total 8 Qu				2950

6. Delays and suggestions.

I ask you to prolongate the project period until October 15th 2005 since two project participants has to perform missions in September (Prof. V.Lvov to the Warsaw, Poland and N.Glavatska – October 2-9th to Partenit, Ukraine), i.e. after determined project end date. Due to that's assignments could be reported and included to the final financial project report.
Prolongation does not need any additional costs. According to this, I ask to prolongate the term for the final financial report, as well as Ff and Sf reports, that includes financial information and reports on the assignments and international contacts.

N.Glavatska

Project Manager